

Asymptotic Expansions with Error Bounds for Solutions of Linear Recurrences

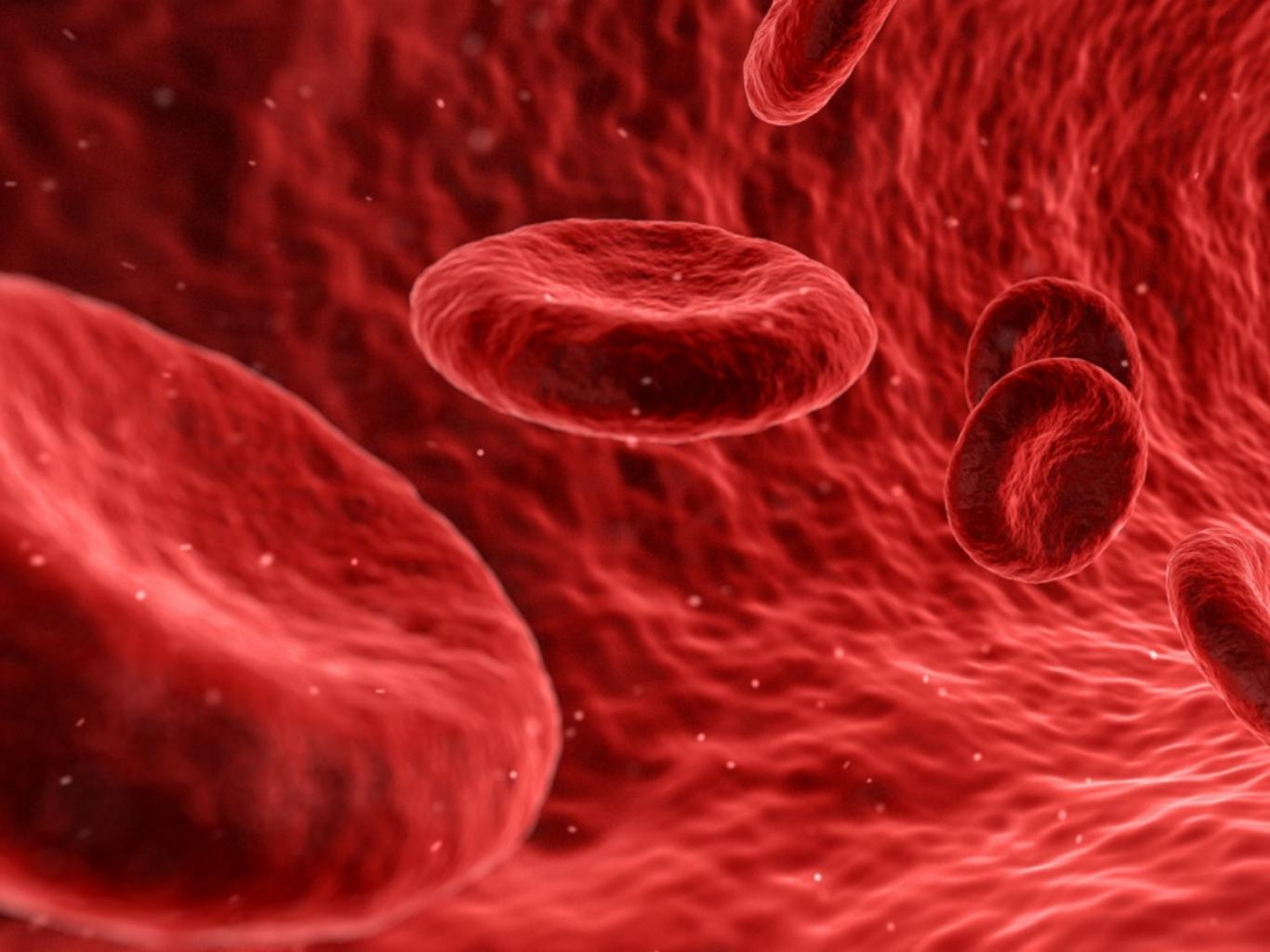
Marc Mezzarobba

CNRS, LIX (Palaiseau)

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

AriC/NuSCAP Seminar, June 15, 2023

arXiv:2212.11742 [cs.SC]



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 (1964b) 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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The Minimum Energy of Bending as a Possible Explanation of the Biconcave Shape of the Red Cell

Universität Regensburg

Willmore Energy

$$\frac{1}{4} \int_S (\kappa_1 + \kappa_2)^2 + \text{cst}_g$$

$\underbrace{}_{W(S)}$

Blood Cell

Canada

Canham Model:

Lindström (1963)
Min. W given g, area, volume

equilibrium form within
a fraction of a second after emerging from very small blood vessels. Rand (1964b) 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.

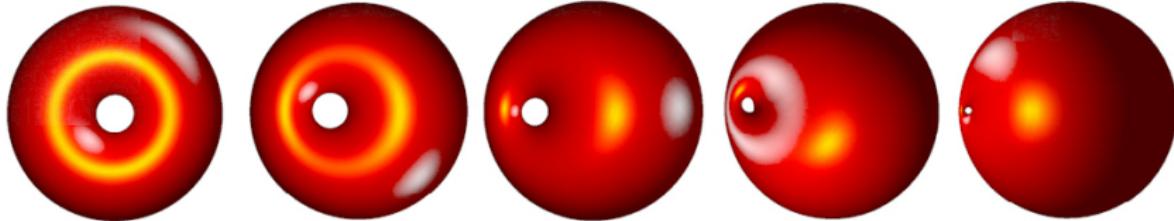
From Minimal Surfaces to Recurrences

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* $\mathbb{T}_C = \mathbb{S}_{1/\sqrt{2}}^1 \times \mathbb{S}_{1/\sqrt{2}}^1 \subset \mathbb{S}^3$



(Yu & Chen 2022)

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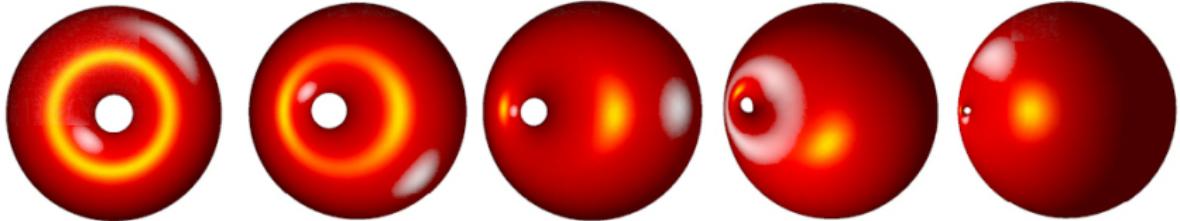
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Unique minimizer (up to scale) of given

$$\text{isoperimetric ratio } \pi^{1/6} (6 V)^{1/3} A^{-1/2} \in [\tau_0, 1)$$

(→ Canham problem)



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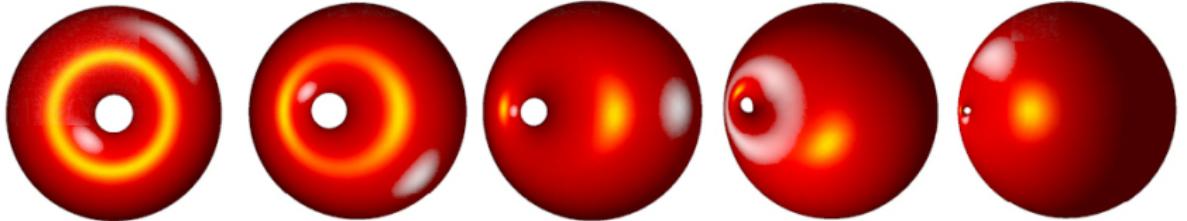
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Unique minimizer (up to scale) of given *isoperimetric ratio* $\pi^{1/6} (6 V)^{1/3} A^{-1/2} \in [\tau_0, 1]$ (\rightarrow Canham problem)

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



(Yu & Chen 2022)

Yu and Chen's Sequence

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

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



Asymptotic behavior

Eventual Positivity

$$\dots d_{n+6} + \dots + \dots d_{n+1} + \dots d_n = 0$$

Routine Calculation

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

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- (among others)

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Corollary

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

Question

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

Complete Positivity

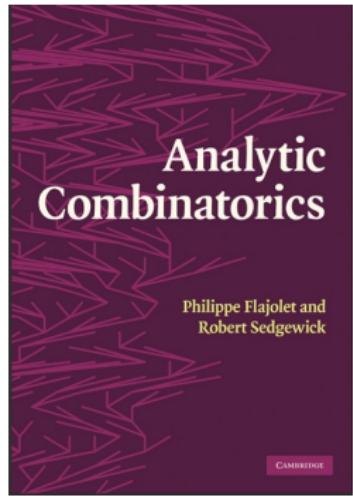
Proposition

[Melczer & M. (2022)]

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

Corollary

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



Complete Positivity

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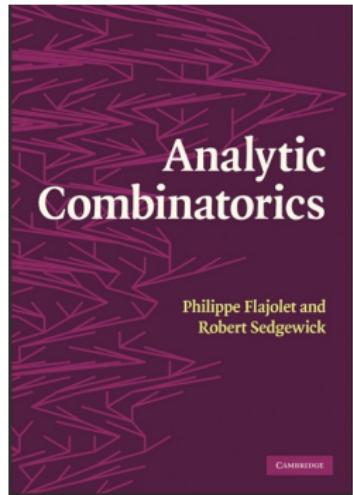
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Real point: We now have the technology
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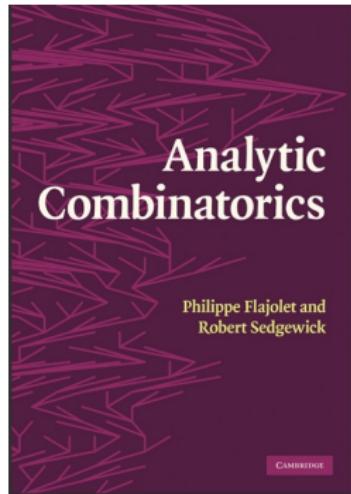
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Next Step

[Dong (2021); Dong, Melczer & M. (2022)]

“General” sequences — Algorithm +  Code

- ▶ van der Hoeven (2021) — Theoretical algorithms using Mellin transforms, complexity



Positivity: Some Related Work

Decidability issues

Induction + CAD

Symbolic-
numeric

Constant coefficients

- ▶ Ouaknine, Worrell (2014)
- ▶ Kenison, Nieuwveld, Ouaknine, Worrell (2023)

- ▶ Nuspl & Pillwein (2022)

Polynomial coefficients

- ▶ Neumann, Ouaknine, Worrell (2021)
- ▶ Kenison, Klurman, Lefacheux, Luca, Moree, Ouaknine, Whiteland, Worrell (2021)

- ▶ Gerhold, Kauers (2005)
- ▶ Kauers, Pillwein (2010)
- ▶ Pillwein (2013)

- ▶ van der Hoeven (2021)
- ▶ Ibrahim, Salvy (2023)

General Recurrences

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

$$\downarrow \quad d(z) = \sum_n d_n z^n$$

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

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Assumptions

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

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

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

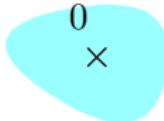
A Cauchy Integral

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

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$$d(z) = 72 + 1932z + 31248z^2 + \dots$$

$$\begin{matrix} 0 \\ \times \end{matrix}$$



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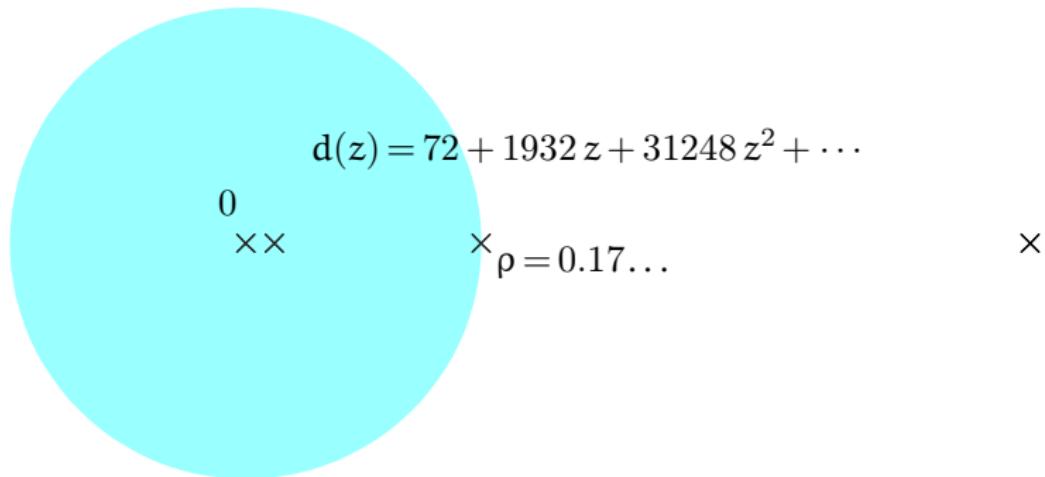
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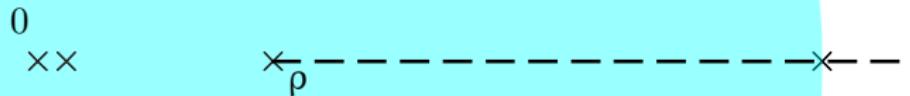


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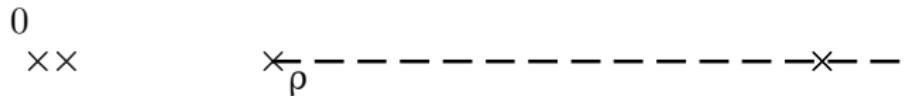
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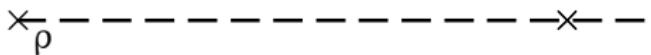
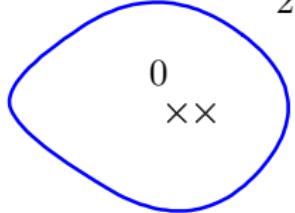


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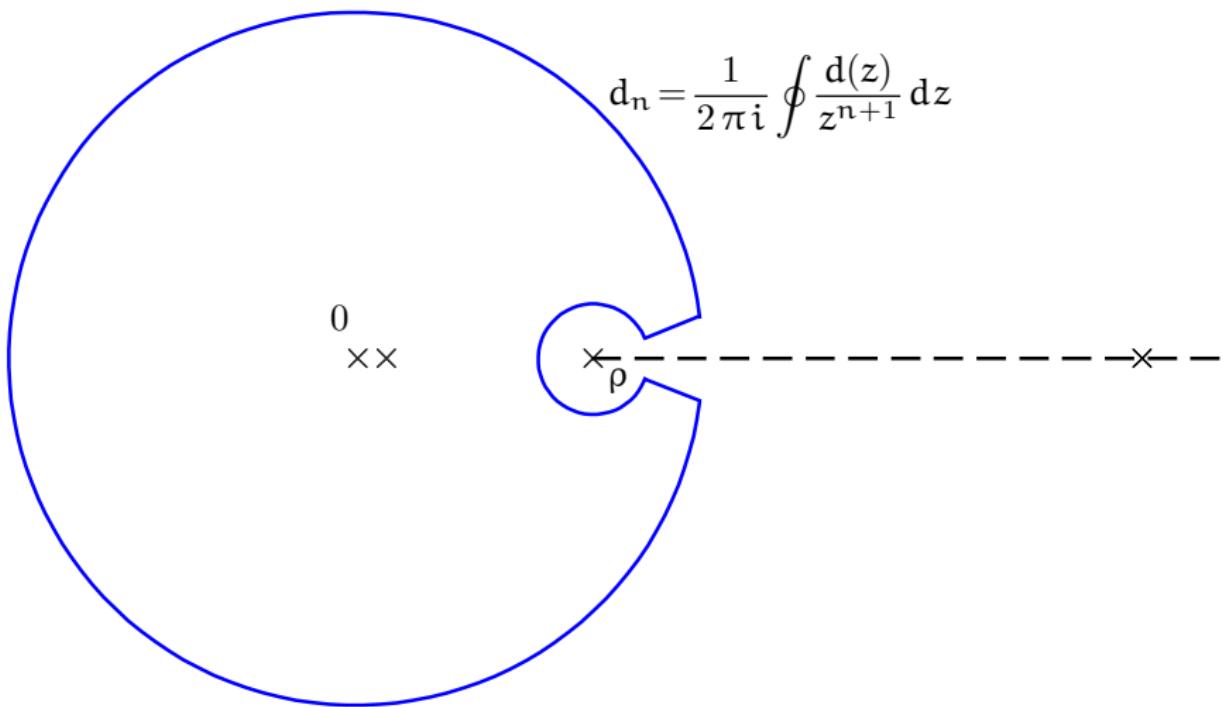


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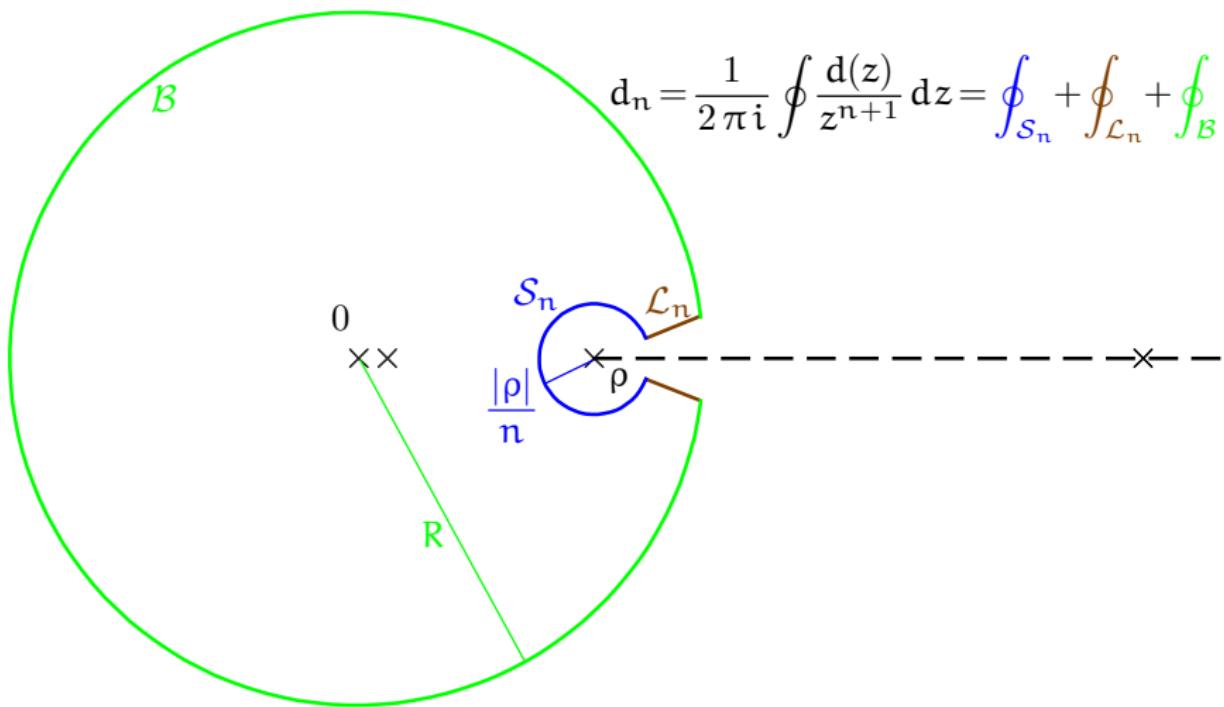
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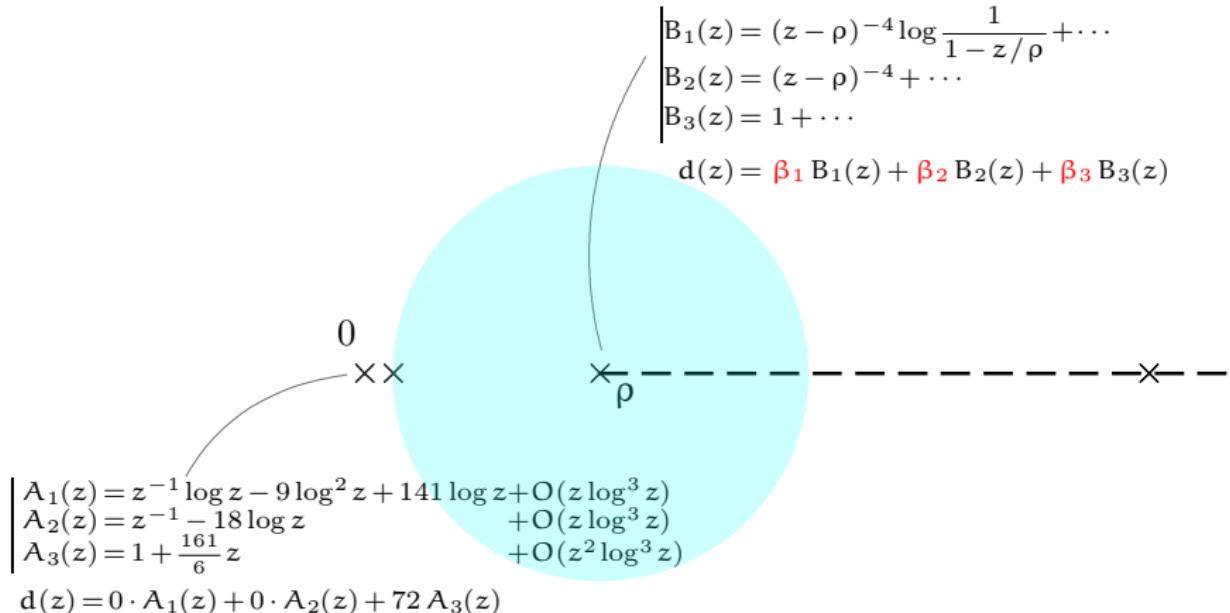
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$$\left| \begin{array}{l} A_1(z) = z^{-1} \log z - 9 \log^2 z + 141 \log z + O(z \log^3 z) \\ A_2(z) = z^{-1} - 18 \log z + O(z \log^3 z) \\ A_3(z) = 1 + \frac{161}{6} z + O(z^2 \log^3 z) \end{array} \right.$$
$$d(z) = 0 \cdot A_1(z) + 0 \cdot A_2(z) + 72 A_3(z)$$

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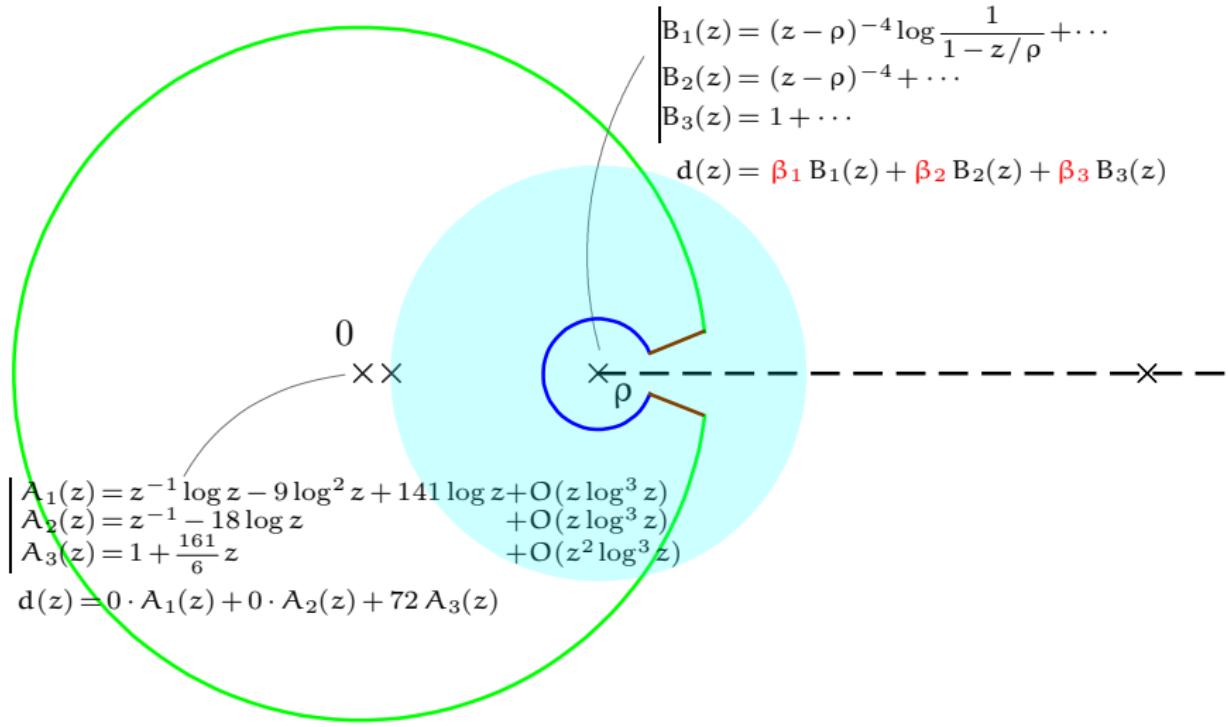
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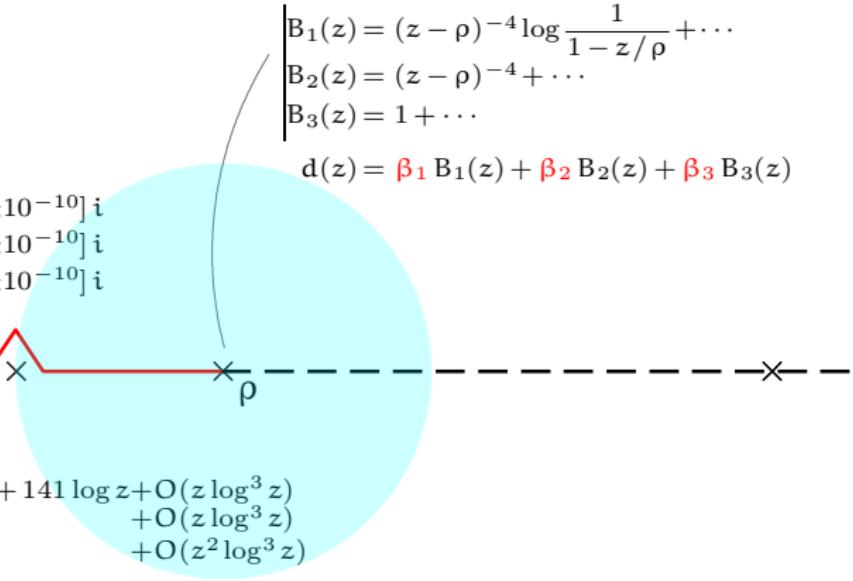


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$$\begin{aligned}\beta_1 &= [0.0420 \pm 10^{-4}] + [\pm 10^{-10}] i \\ \beta_2 &= [0.0598 \pm 10^{-4}] + [\pm 10^{-10}] i \\ \beta_3 &= [0.7302 \pm 10^{-4}] + [\pm 10^{-10}] i\end{aligned}$$



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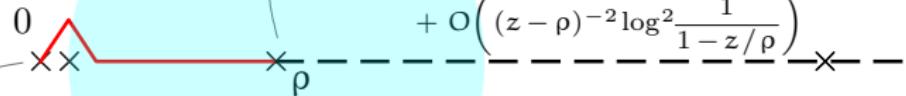
$$B_1(z) = (z - \rho)^{-4} \log \frac{1}{1 - z/\rho} + \dots$$

$$B_2(z) = (z - \rho)^{-4} + \dots$$

$$B_3(z) = 1 + \dots$$

$$\begin{aligned} d(z) &= \beta_1 B_1(z) + \beta_2 B_2(z) + \beta_3 B_3(z) \\ &= [0.0420 \pm 10^{-4}] (z - \rho)^{-4} \log \frac{1}{1 - z/\rho} \\ &\quad + [0.0598 \pm 10^{-4}] (z - \rho)^{-4} \\ &\quad - [0.0209 \pm 10^{-4}] (z - \rho)^{-3} \log \frac{1}{1 - z/\rho} \\ &\quad + [0.0491 \pm 10^{-4}] (z - \rho)^{-3} \\ &\quad + O\left((z - \rho)^{-2} \log^2 \frac{1}{1 - z/\rho}\right) \end{aligned}$$

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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 $\{f(z) : z \in \boxed{z}\}$

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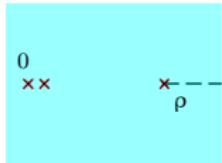
Bounds on Tails of Logarithmic Series

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

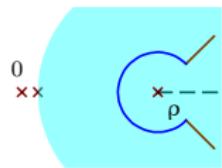
$$A(z) = (z - \rho)^\nu \sum_{k=0}^K \left(\sum_{n=0}^{N-1} u_{n,k} (z - \rho)^n + \underbrace{\sum_{n=N}^{\infty} u_{n,k} (z - \rho)^n}_{|\cdot| \leq \mathbf{M}_k |z - \rho|^N \text{ for } |z - \rho| \leq \delta} \right) \log^k \frac{1}{1 - z/\rho}$$

Singular Expansion

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

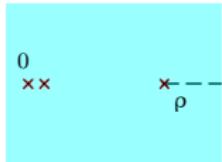


$$+ \underbrace{\sum_{n=\nu+r}^{\infty} \left[c_{n,0} + c_{n,1} \log \frac{1}{z-\rho} + c_{n,2} \log^2 \frac{1}{z-\rho} \right] (z-\rho)^n}_{g(z)} \\ (\nu = -4, r = 2)$$

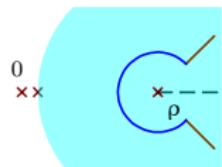


Singular Expansion

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

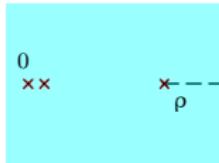


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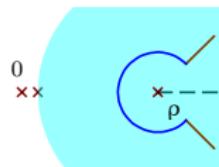


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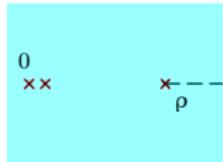
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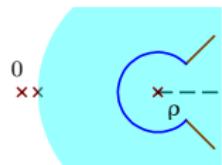
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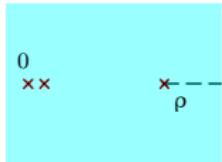
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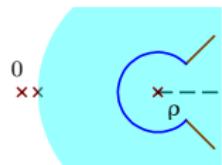
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Bound each term for $n \geq n_0$

The Explicit Part (I)

[Jungen 1931, ...]

$$\begin{aligned}[z^n] (1-z)^\alpha \log^k \frac{1}{1-z} &= \frac{d^k}{d\alpha^k} \binom{n+\alpha-1}{n} \quad (\rho=1) \\ &= \underbrace{\frac{\Gamma(n+\alpha)}{\Gamma(n+1)}}_{G(n)} \underbrace{\frac{1}{\Gamma(n+\alpha)} \frac{d^k}{d\alpha^k} \frac{\Gamma(n+\alpha)}{\Gamma(\alpha)}}_{H(n,k)}\end{aligned}$$

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Lemma (Gamma ratios)

Corollary of [Frenzen 1992]

For $n > |\alpha|$,

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

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

... = explicit coefficients
in terms of generalized Bernoulli numbers

C_{α, r, n_0} = explicit constant

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

\dots = explicit coefficients
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The Explicit Part (II)

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

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Lemma

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

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

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Theorem

[Nemes 2017]

For $|\arg z| \leq \pi/4$

$$\psi^{(0)}(z) = \log z - \sum_{j=0}^{r-1} \frac{\dots}{z^j} + R(z), \quad |R(z)| \leq C_{0,r} |z|^{-r}$$

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

The Explicit Part: Summary

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

$$[z^n] \ell(z)$$

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$$[z^n] (z - \rho)^{-\alpha} \log^k \frac{1}{z - \rho}$$


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

$$\begin{aligned} & [z^n] (z - \rho)^{-\alpha} \log^k \frac{1}{z - \rho} \\ &= \rho^{-n} n^{\alpha-1} \left(\square \log^k n + \square \log^{k-1} n + \cdots + \square \right. \\ &\quad \left. + \square \frac{\log^k n}{n} + \cdots + \square \frac{1}{n} \right. \\ &\quad \left. + \cdots \right. \\ &\quad \left. + R(n) \right) \end{aligned}$$

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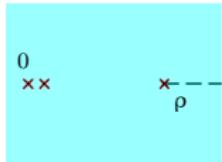
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$$\begin{aligned}[z^n] \ell(z) = \rho^{-n} \left([8.07 \pm 10^{-3}] n^3 \ln n + [1.37 \pm 10^{-3}] n^3 \right. \\+ [50.5 \pm 10^{-1}] n^2 \ln n + [29.7 \pm 10^{-1}] n^2 \\+ [\pm 1.5 \cdot 10^3] n \ln^2 n \left. \right)\end{aligned}$$

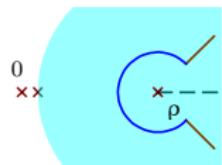
for all $n \geq 50$

Singular Expansion

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



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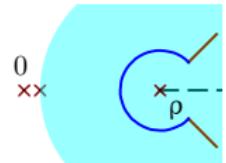


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Bound each term for $n \geq n_0$

The Local Error Term

$$g(z) = (z - \rho)^{\nu+r} \left(h_0(z) + h_1(z) \log \frac{1}{z - \rho} + h_2(z) \log^2 \frac{1}{z - \rho} \right)$$



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 $\{f(z) : z \in \boxed{z}\}$

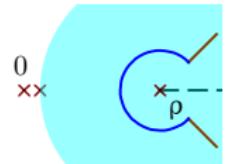
Bounds on Tails of Logarithmic Series

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

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

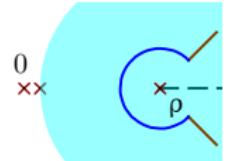
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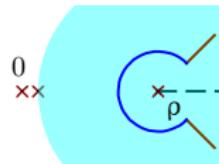
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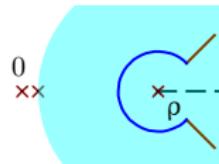
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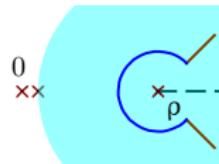
$$B(z) = B_0 + B_1 z + B_2 z^2 \quad \left| \log \frac{1}{1 - z/\rho} \right| \leq \pi + \log n \quad \text{on } \mathcal{S}_n$$

Lemma (Error term on the small arc)

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

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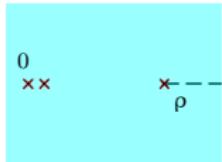
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Lemma (Error term on the line segments)

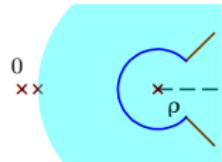
$$\lim_{\varphi \rightarrow 0} \left| \frac{1}{2\pi i} \int_{\mathcal{L}_n} \frac{g(z)}{z^{n+1}} dz \right| \leq C'_{\rho, \nu, r} |\rho|^{-n} n^{-\operatorname{Re}(\nu)-1-r} B(\pi + \log n)$$

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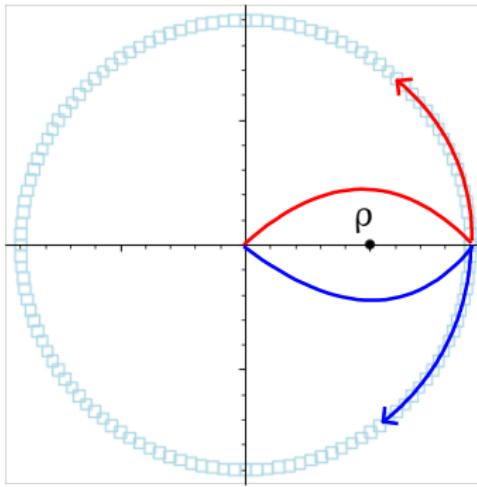


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Bound each term for $n \geq n_0$

The Global Error Term

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



compute $d(z)$ using the diff. eq.
(staying in the analyticity domain of $d(z)!$)

Conclusion

“Generic Case”

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

$n \geq 50$

Conclusion

“Generic Case”

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

$n \geq 50$

What may go wrong

► Multiple dominant singularities

$$2^n \left(\square + \frac{\square}{n} \right) + (-2)^n \left(\square + \frac{\square}{n} \right) + [\pm M] \frac{1}{n^2}$$

- not an asymptotic expansion
- still makes sense as a bound

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- ▶ Failure to detect exact zeros $2^n \left([\pm 10^{-100}] + \dots \right) + [12.3 \pm 10^{-1}] + \frac{[4.56 \pm 10^{-1}]}{n}$
 - ▶ useless bound (for large n)
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- ▶ Irregular singular points

Image Credits

- ▶ Red blood cells

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