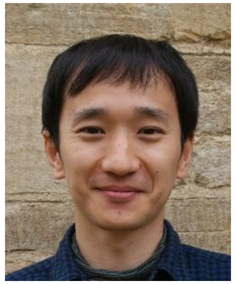
Approximation on complex domains and Riemann surfaces

Nick Trefethen, University of Oxford

Abi Gopal



Yuji Nakatsukasa

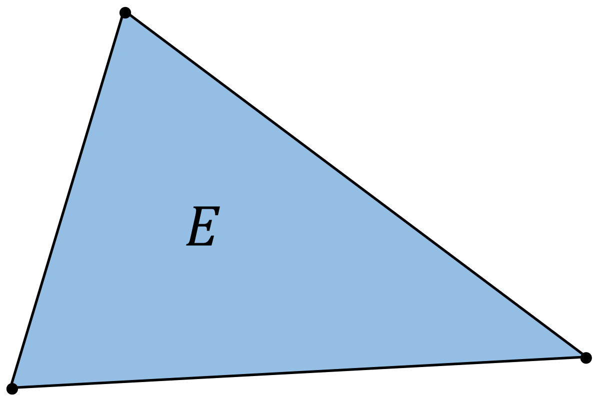
André Weideman

0. A personal remark
1. The problem, and a numerical demonstration
2. From one to several corners via Cauchy integrals ← *question*
3. Root-exponential convergence of rational approximations
4. Exponential-minus-log convergence of reciprocal-log approximations
5. Riemann surfaces

1. The problem, and a numerical demonstration

Given:

- Closed Jordan region E with piecewise analytic boundary.
- Continuous function f analytic on E except for branch point singularities at the corners.



Typically these involve fractional powers and logs, and we assume f is analytically continuable along curves winding around the branch points.

Problem:

- Approximate f by simple functions r_n depending on n parameters, with rapid convergence as $n \to \infty$.

Polynomials are useless: terribly slow convergence. Our aim is:

Root-exponential convergence: $\|f - r_n\| = O(\exp(-C\sqrt{n}\,))$

Exponential-minus-log convergence: $\|f - r_n\| = O(\exp(-Cn/\log n))$.

$$\|\cdot\| = \|\cdot\|_\infty,\ C > 0,\ n \to \infty.$$

Motivation

Numerical solution of PDEs in domains with corners, starting with the Laplace equation.

Solutions typically have branch point singularities at the corners. (Lehman 1957, Wasow 1957)

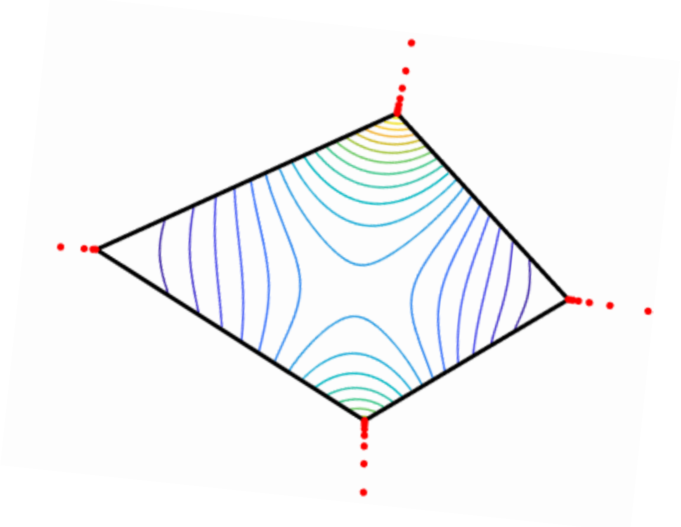
"Lightning Laplace solver" (Gopal & T., *SINUM* 2019 and *PNAS* 2019)

$$r(z) = \sum_{j=1}^{n_1} \frac{a_j}{z - z_j} + p_{n_2}(z)$$

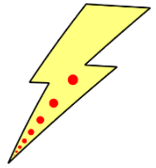
(1) Fix poles exponentially clustered near each corner.

(2) Fit the boundary data by the real part of a rational function with these poles (discrete least-squares fitting in thousands of sample points, also clustered near the corners).

(3) This gives the solution in the interior, typically accurate to 6-10 digits.



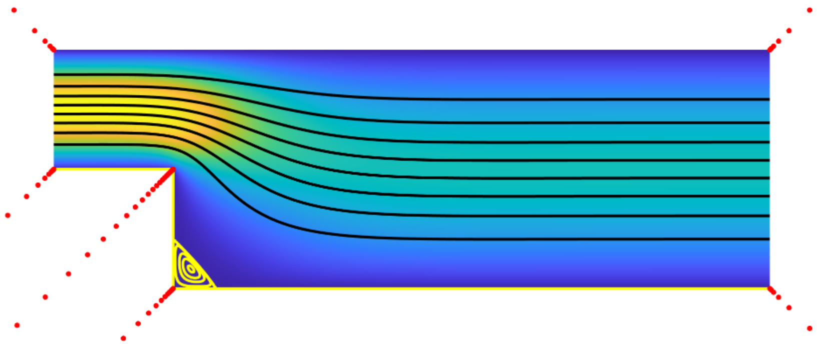
```
laplace('L');
laplace('L', 'tol', 1e-10);
laplace('iso');
laplace(8);
laplace(-8);

confmap('L');
```



Codes: `https://people.maths.ox.ac.uk/trefethen/lightning.html.`

Lightning Stokes solver

(Brubeck & T., work in progress)



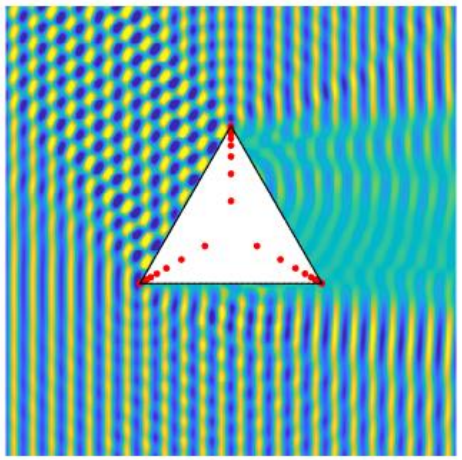
Biharmonic eq. $\Delta^2 u = 0.$

Reduce to Laplace problems via Goursat representation $u = \mathrm{Re}(\,\overline{z} f + g).$

Root-exponential convergence to 10 digits.

Lightning Helmholtz solver

(Gopal & T., *PNAS*, 2019)



Helmholtz eq. $\Delta u + k^2 u = 0.$

Instead of sums of simple poles $\left(z - z_j\right)^{-1}$, use sums of complex Hankel functions $H_1\left(k\left|z - z_j\right|\right)\exp(\pm i \arg(z - z_j)).$

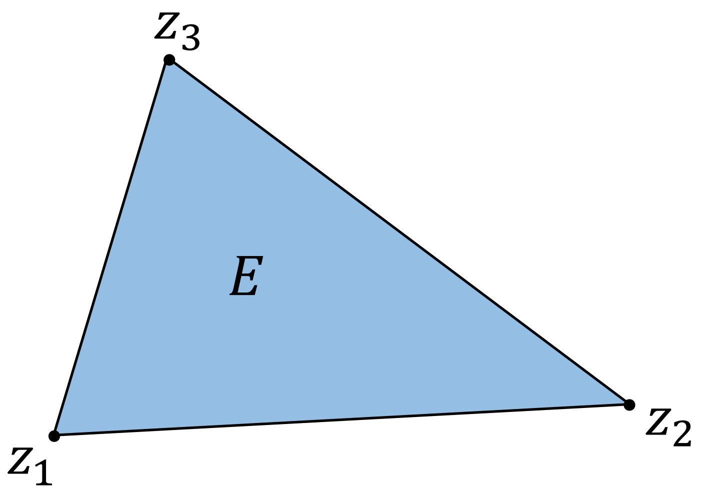
Root-exponential convergence to 10 digits.

No theory as yet.

2. From one to several corners via Cauchy integrals

Computationally, this is a non-issue. Least-squares works for several corners just as for one.

Theoretically, however, there is a challenge.
Suppose we can prove existence of good approximations locally near one singularity.
How can we prove they exist globally on E with m singularities?



Idea 1: decompose f via partition of unity

Not good. Hard to ensure enough smoothness of the partition.

Idea 2: approximate f separately near each corner

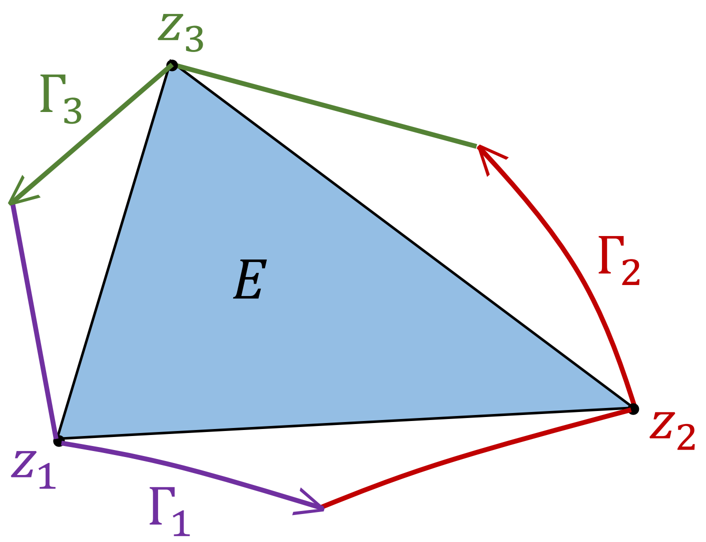
(1) Find f_k with $f_k \approx f$ near z_k, analytic elsewhere on E.

(2) Then $\sum f_k - f$ is $\approx$ analytic on E, hence easily approximable.

This fails at step (1). By uniqueness of analytic continuations,
f_k would have to approximate the other singularities too.

Instead we have used *Idea 3: decompose f via Cauchy integrals over open arcs*.

Decomposing f via Cauchy integrals over open arcs



Write $f = f_1 + \cdots + f_m$ with $f_k(z) = \dfrac{1}{2\pi i}\displaystyle\int_{\Gamma_k} \dfrac{f(t)}{t-z}\,dt$.

f_k inherits the singularity of f at z_k but not at the other corners, for it is analytic throughout $\mathbb{C} \setminus \Gamma_k$.

With this decomposition we readily extend approximation theorems to domains with m corners.

Question. Is this the right thing to do? If so, it has surely been done before. Where? By whom?

3. Root-exponential convergence of rational approximations

Donald Newman 1964:

$O(\exp(-C\sqrt{n}\,))$ convergence for degree n rational best approximation of $|x|$ on $[-1,1]$, with exponential clustering of poles near 0. Equivalent problem: approximation of $\sqrt{x}$ on $[0,1]$.

A great deal of approximation theory has followed, mainly focused on best (minimax) approximations. Key tool: Hermite contour integral formula for rational interpolants.

(Walsh, Gonchar, Rakhmanov, Stahl, Saff, Totik, Aptekarev, Suetin)

What's new

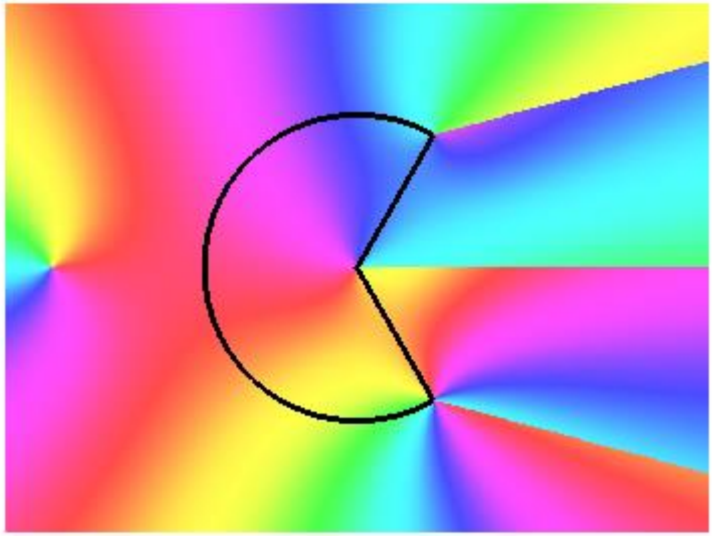
- Extension of root-exponential result to domains with m corners (Gopal & T., *SINUM* 2019)
- AAA algorithm for fast near-best approx with free poles (Nakatsukasa-Sète-T., *SISC* 2018)
- Lightning algorithm for linear approx with fixed exponentially clustered poles (Gopal & T., *SINUM* 2019)

(Plus a few other things too. Ask me afterwards.)

Phase portrait of a function f with three corner singularities

(Wegert book, 2012)

f

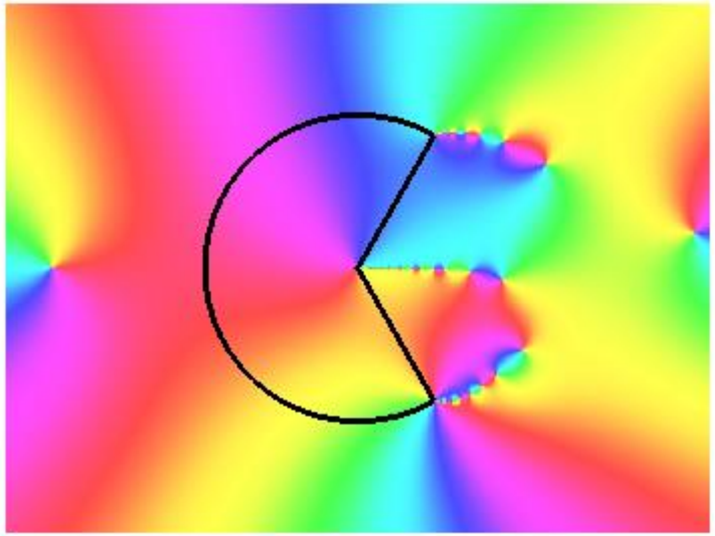


$$f(z) = z\log(-\tfrac{1}{2}z)\cdot(1 - z/\omega)^{1/2}\cdot(1 - z/\bar{\omega})^{3/2}$$

$$\omega = e^{\pi i/3}$$

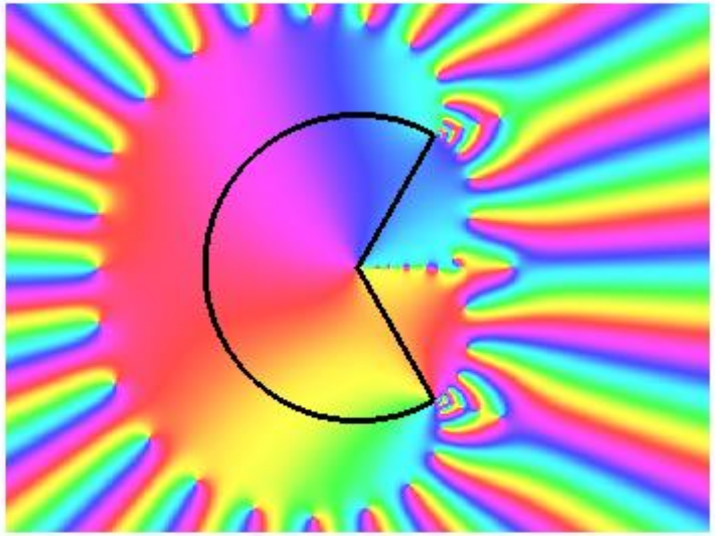
AAA and lightning rational approximations

AAA



free poles, adaptively determined

lightning



preassigned poles, exponentially clustered

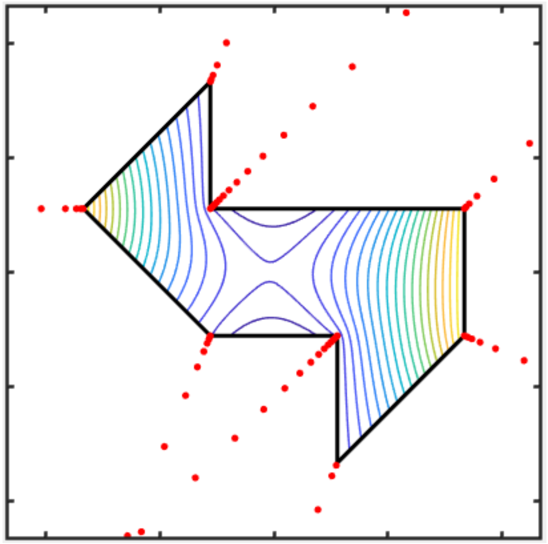
Theorem on lightning approximation

(Thm. 2.3 of Gopal & T., *SINUM* 2019)

$$r(z) = \sum_{j=1}^{n_1} \frac{a_j}{z - z_j} + p_{n_2}(z)$$

n parameters in total

Theorem. $\|f - r_n\|_E = O(\exp(-C\sqrt{n}\,))$



f has Hölder continuous branch point singularities at the corners.

r_n has fixed exponentially clustered poles;
the precise formula is quite flexible.

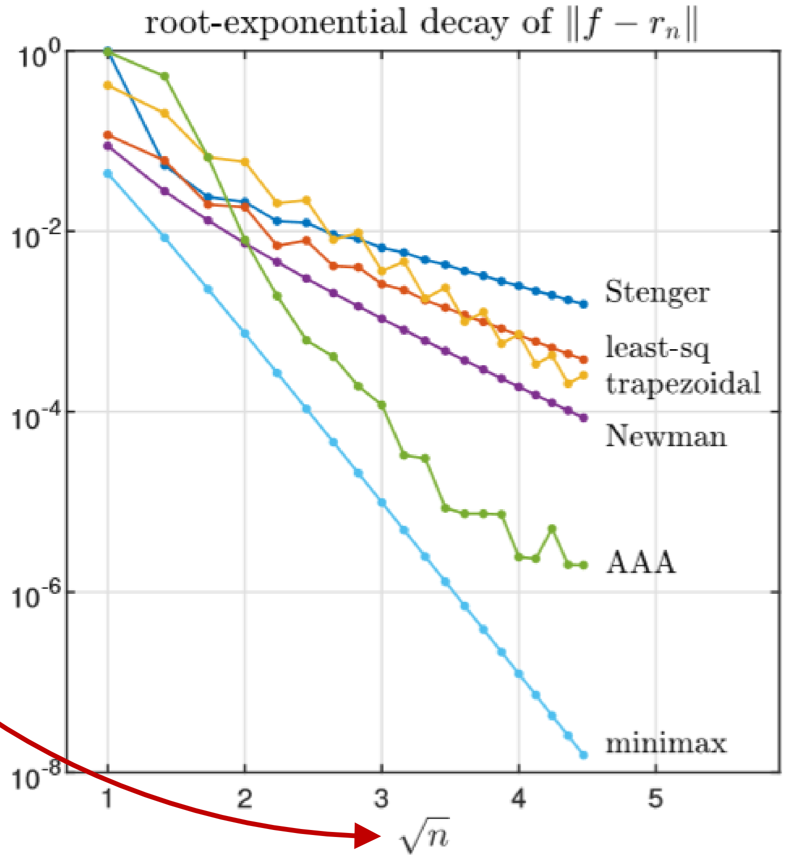
Proof: Hermite integral formula + Cauchy integral decomposition.

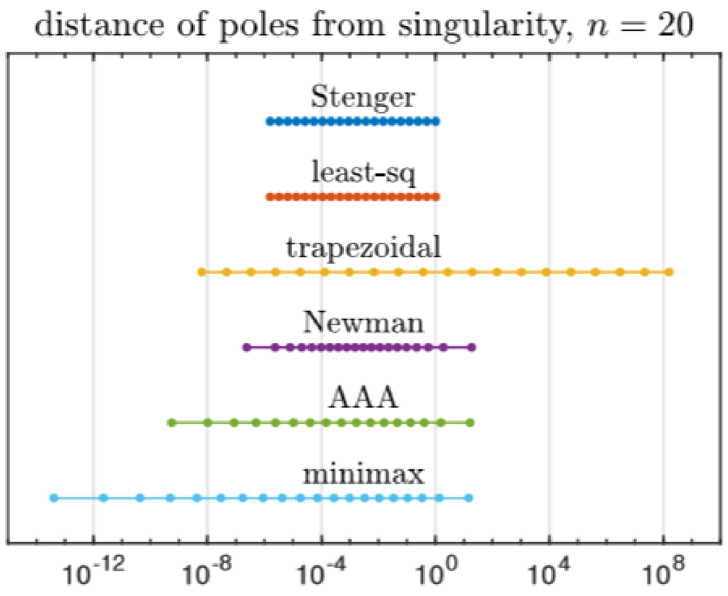
Assume E is convex, but probably not needed by potential theory.

Six rational approximations of $\sqrt{x}$ on $[0,1]$

The figures on this and the next two slides are from T.-Nakatsukasa-Weideman, *Numer. Math.* to appear.

root-exponential convergence



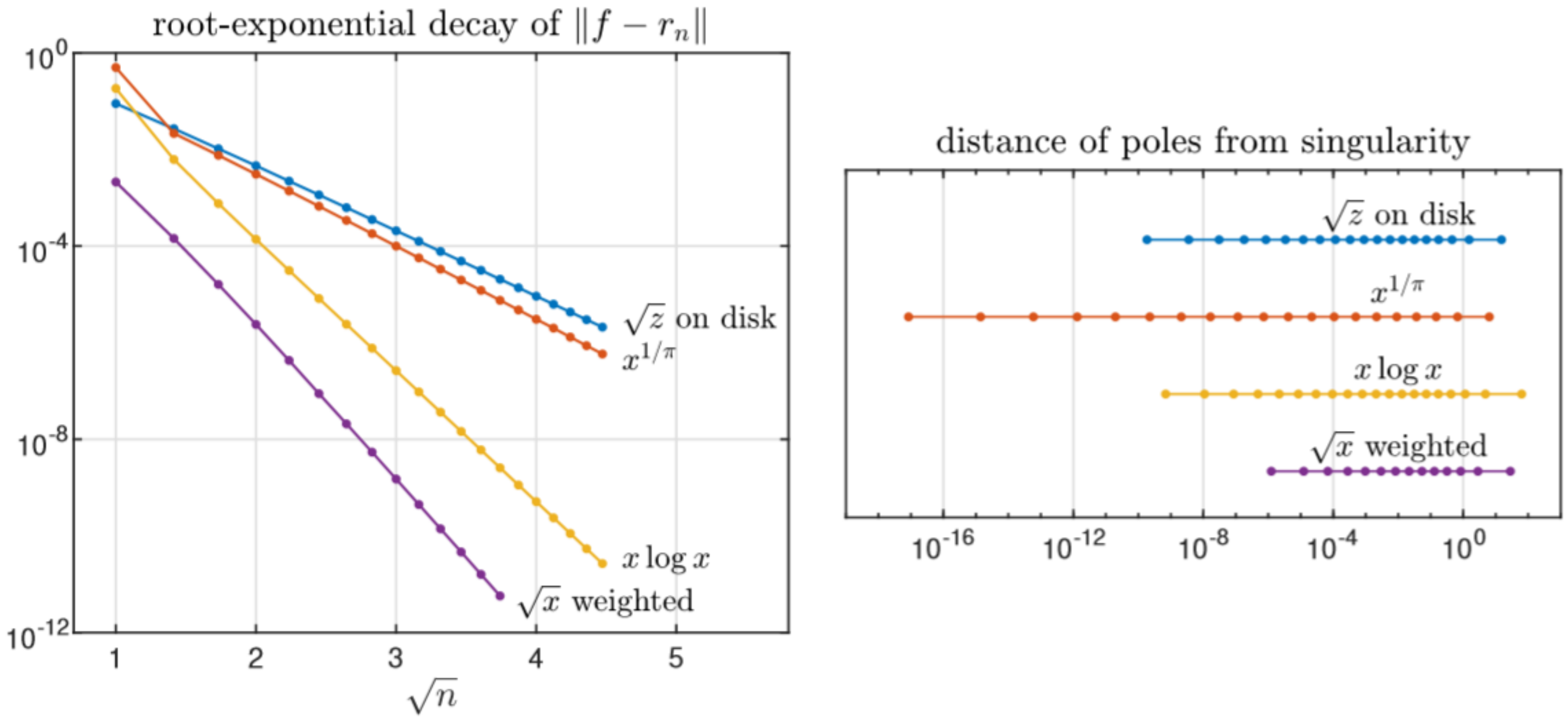


exponential clustering of poles

Fig. 1 Root-exponential convergence of six kinds of degree n rational approximations of $f(x) = \sqrt{x}$ on $[0,1]$ as $n \to \infty$. On the upper-left, the asymptotically straight lines on this log scale with $\sqrt{n}$ on the horizontal axis (except for AAA) show the root-exponential effect. On the upper-right, the distances of the poles in $(-\infty, 0)$ from the singularity at $x = 0$ show the exponential clustering.

Four minimax rational approximation problems

root-exponential convergence

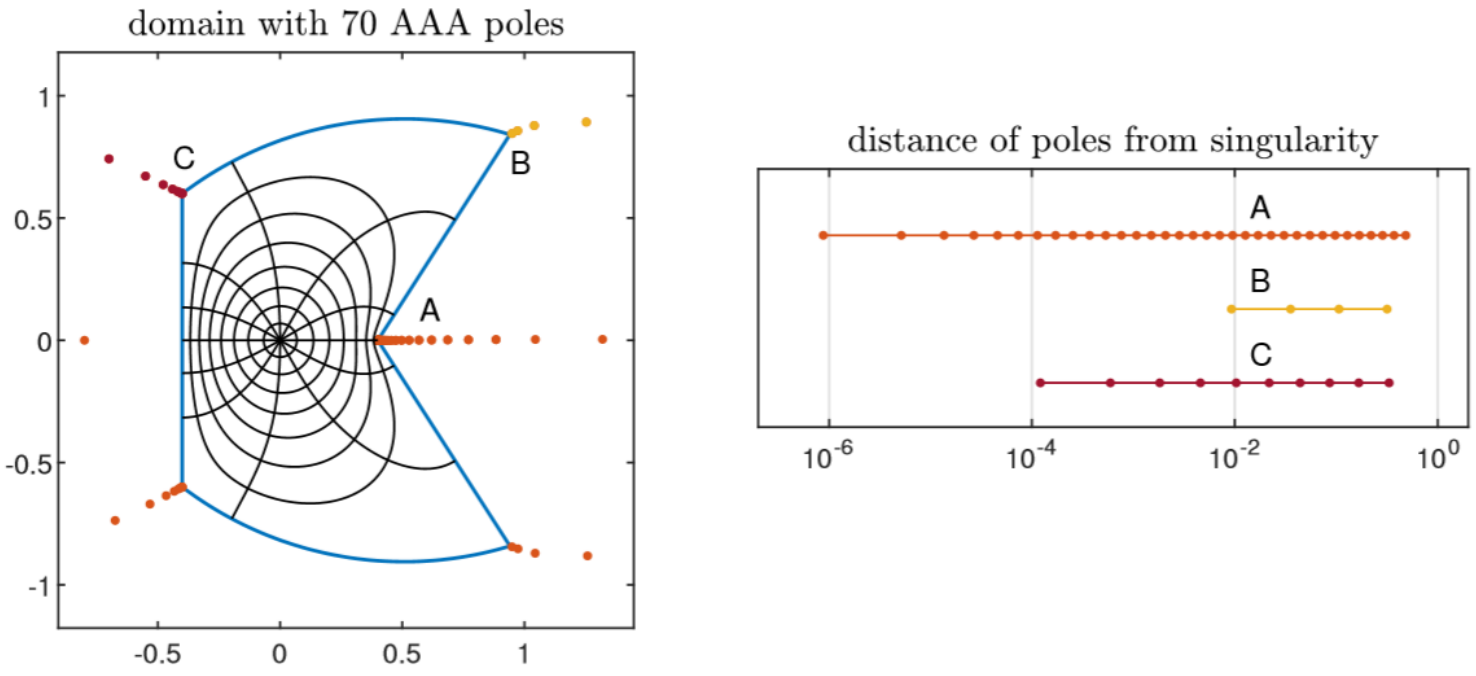


exponential clustering of poles

Fig. 2 Four more minimax approximations, showing the same root-exponential convergence and exponential clustering of poles as in Fig. 1. Two involve the functions $x^{1/\pi}$ and $x \log x$ on $[0, 1]$, one involves x on $[0, 1]$ but with the ∞-norm weighted by x, and one involves $\sqrt{z}$ on the disk about $\frac{1}{2}$ of radius $\frac{1}{2}$. In the right image, n takes its final value from the left image for each problem, 14 for the weighted approximation and 20 for the other cases.

AAA rational approximation of a conformal map

NB: These are free poles, chosen adaptively by AAA.



exponential clustering of poles

Fig. 3 The conformal map of a circular pentagon onto the unit disk has been computed and then approximated numerically by a rational function of degree 70 [13, 57] by the AAA algorithm. The poles cluster exponentially at the corners, where the map is singular.

4. Exponential-minus-log convergence of reciprocal-log approximations

A new idea came along 3½ months ago. (Nakatsukasa & T., *SINUM*, submitted)

Change from rational to reciprocal-log approximation.

Convergence rate may speed up to exponential !

Singularity at 0:
$$g(z) = c_0 + \sum_{k=1}^{n} \frac{c_k}{\log(z) - s_k}$$

Singularities at $z_1, \ldots, z_m$:
$$\boxed{g(z) = \sum_{j=1}^{m} \sum_{k=1}^{n_j} \frac{c_{jk}}{\log(z - z_j) - s_{jk}} + p_0(z)}$$

As ever, the numbers $\{s_{jk}\}$ are fixed in advance in a systematic way and the coefficients $\{c_{jk}\}$ are found by discrete least-squares fitting on the boundary.

Why should this work?

Explanation

Suppose we want to approximate z^a on $[0,1]$.

Change variables: $s = \log(z)$, $z = e^s$.

You get approximation of e^{as} on $(-\infty, 0]$. $\rightarrow$ A famous problem with exponential convergence

(Cody-Meinardus-Varga 1969)

$$\boxed{e^{as} \approx \sum_{k=1}^{n} \frac{c_k}{s - s_k}} \iff \boxed{z^a \approx \sum_{k=1}^{n} \frac{c_k}{\log(z) - s_k}}$$

RATIONAL APROXIMATION ON $(-\infty, 0]$ **RECIPROCAL-LOG APROXIMATION ON** $[0,1]$

Theorems on log-lightning approximation

$$g(z) = \sum_{j=1}^{m} \sum_{k=1}^{n_j} \frac{c_{jk}}{\log(z - z_j) - s_{jk}} + p_0(z)$$

n parameters in total

Approximate $f \approx g_n$ on a simply-connected compact set E in the complex plane.
Assume f can be analytically continued along contours winding around the corners.
With Hermite integral formula + potential theory + Cauchy integral decomposition we show:

1 singularity (Thm. 4.2 of Nakatsukasa & T., *SINUM*, submitted)

Theorem. $\|f - g_n\|_E = O(\exp(-Cn))$ *if* f *is analytic in all of* $\mathbb{C}$ *except for* $\{z_k\}$.

The proof uses points $\{e^{s_k}\}$ growing exponentially with n, which may be confluent.

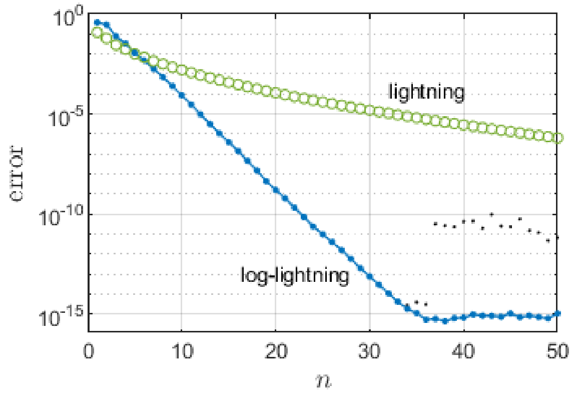
$m \geq 1$ singularities (Thm. 5.1 of Nakatsukasa & T.)

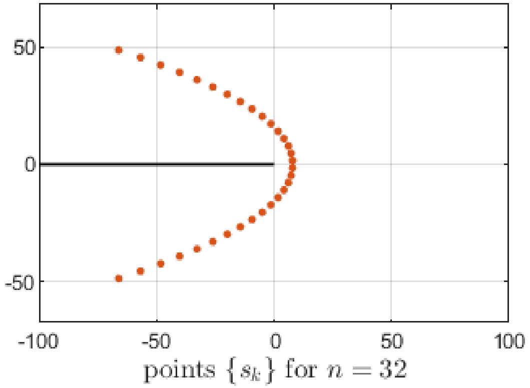
Theorem. $\|f - g_n\|_E = O(\exp(-Cn/\log n))$ *if* f *is analytic in a nbhd of* E *except for* $\{z_k\}$.

The proof uses bounded points $\{e^{s_k}\}$, which lie on $O(n)$ sheets of the Riemann surface of f.
There are some additional technical assumptions.

Log-lightning approximation of $\sqrt{x}$ on $[0,1]$

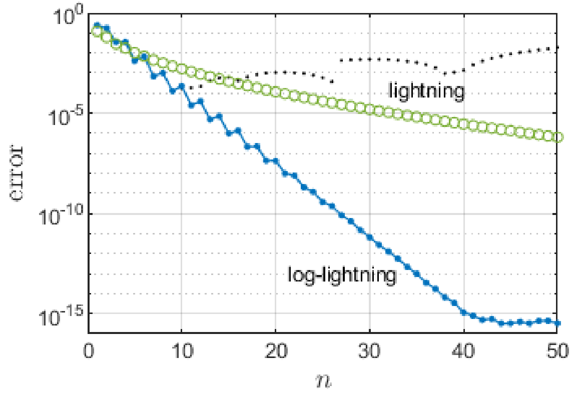
$$g(z) = c_0 + \sum_{k=1}^{n} \frac{c_k}{\log(z) - s_k}$$

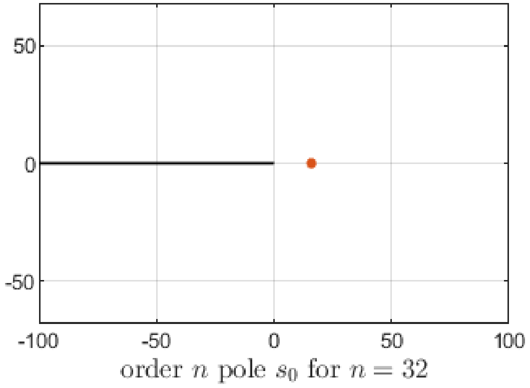




← singularities $\{s_k\}$ on a Hankel contour

(cf. Weideman & T., *Math. Comp.* 2007)





← confluent singularities $\{s_k\}$

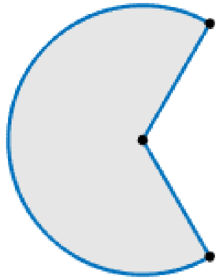
Numerical stability relies on Vandermonde + Arnoldi = Stieltjes orthogonalization (Brubeck-Nakatsukasa-T., *SIREV* to appear).

Black dots show results if you don't stabilize.

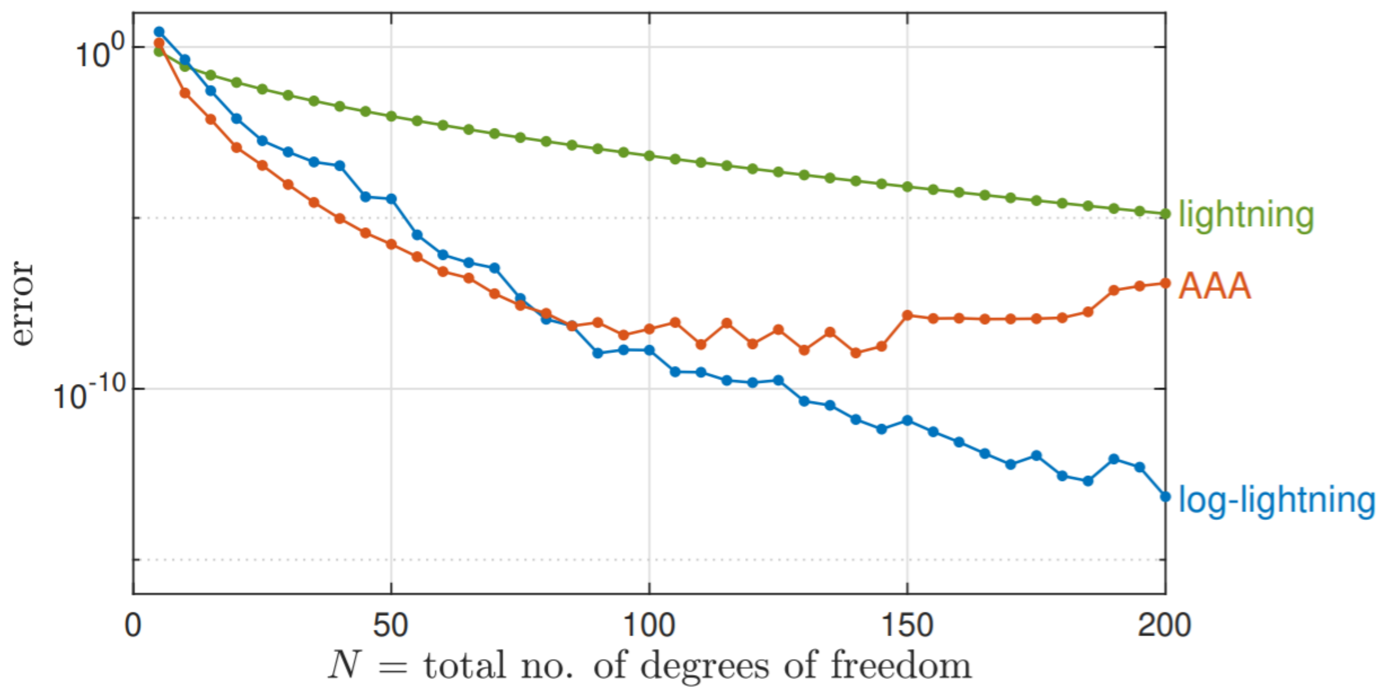
Approximation on a planar region with 3 singularities

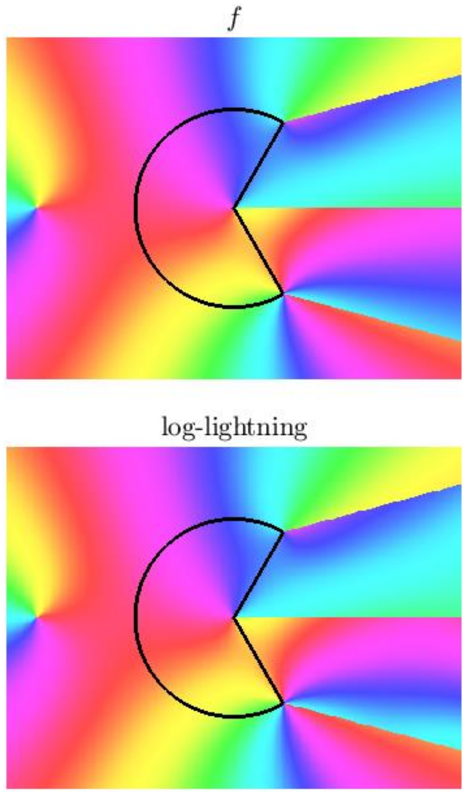
$$\boxed{g(z) = \sum_{j=1}^{m} \sum_{k=1}^{n_j} \frac{c_{jk}}{\log(z - z_j) - s_{jk}} + p_0(z)}$$

(confluent singularities $\{s_k\}$)



$$f(z) = z\log(-\tfrac{1}{2}z) \cdot (1 - z/\omega)^{1/2} \cdot (1 - z/\bar{\omega})^{3/2}, \quad \omega = e^{\pi i/3}$$





Towards a log-lightning Laplace solver

There is no software yet, just one experiment.

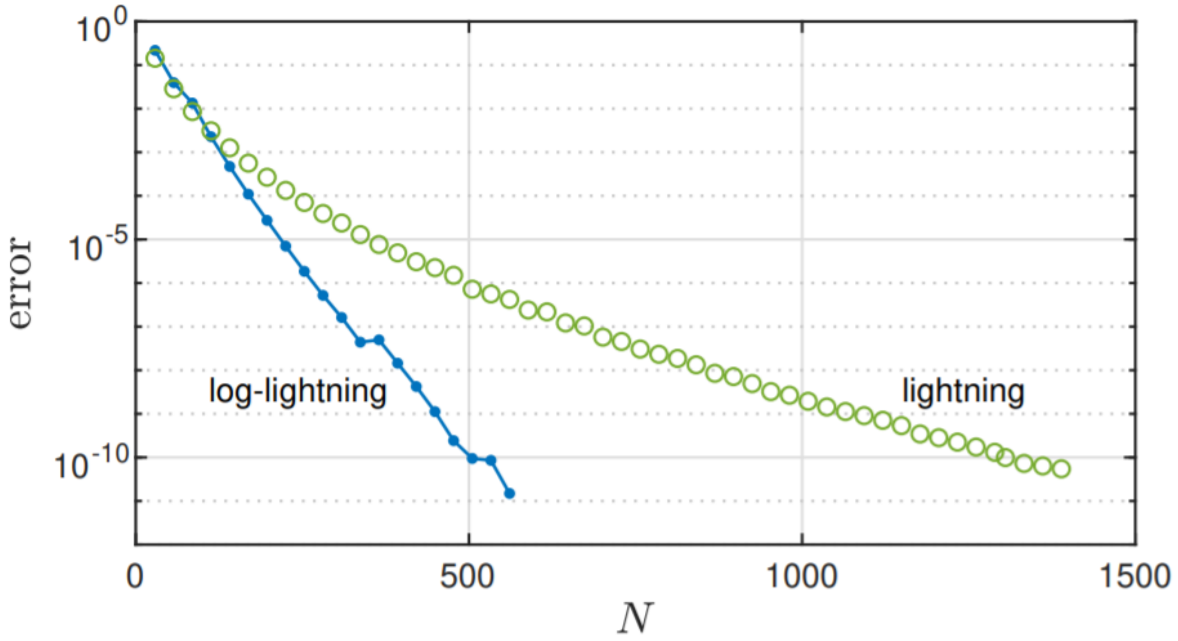
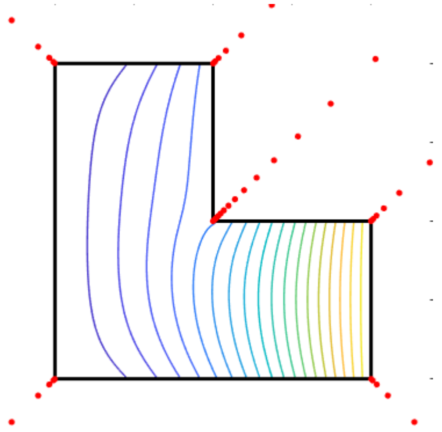


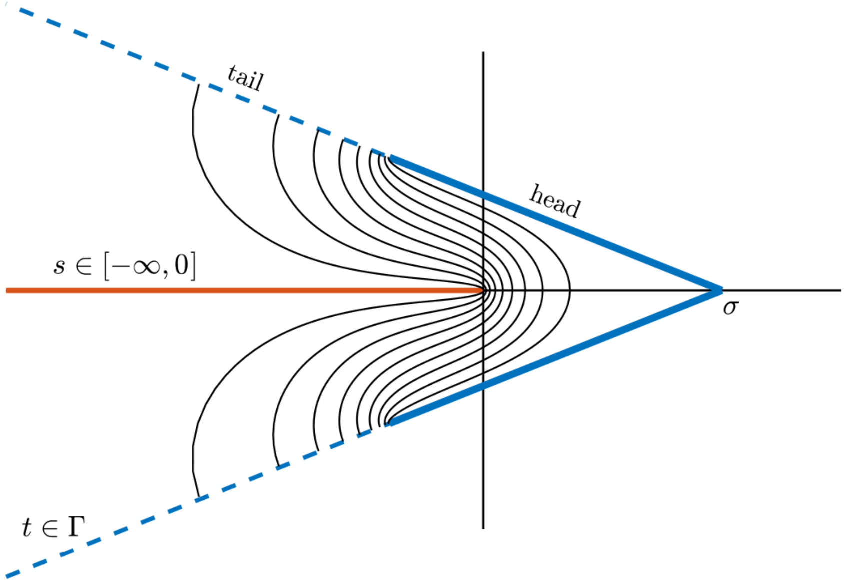
FIG. 7.1. *Convergence of lightning and log-lightning solutions to the NA Digest problem of the Laplace equation on an L-shaped region [18]. The difference between root-exponential and exponential convergence is evident.*



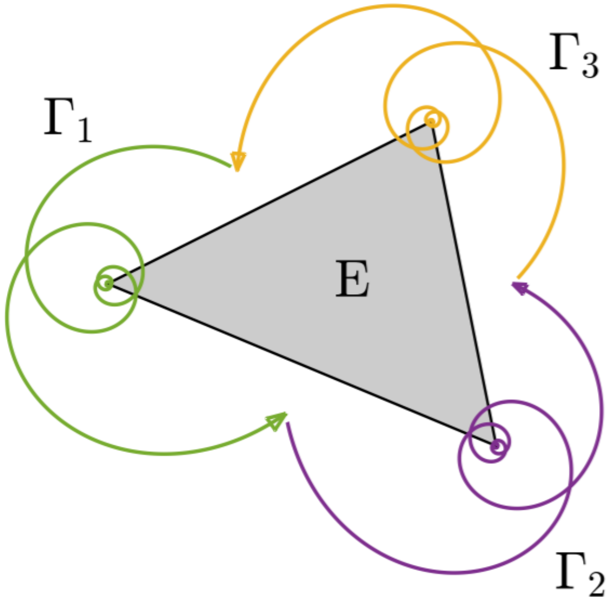
Laplace equation on an L-shaped region

5. Riemann surfaces

Our Hermite integral estimates come from integrals over unbounded V-shaped contours in the $s = \log(z - z_k)$ plane.



In the original z variable, these become logarithmic spirals near each corner.

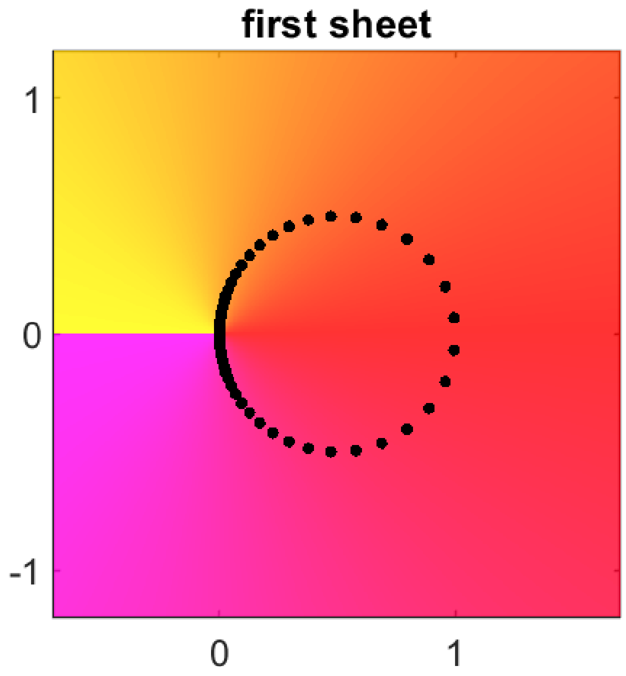


Thus the theory makes use of Riemann surfaces, and the approximations are valid on the Riemann surfaces too. Much to explore here.

Example

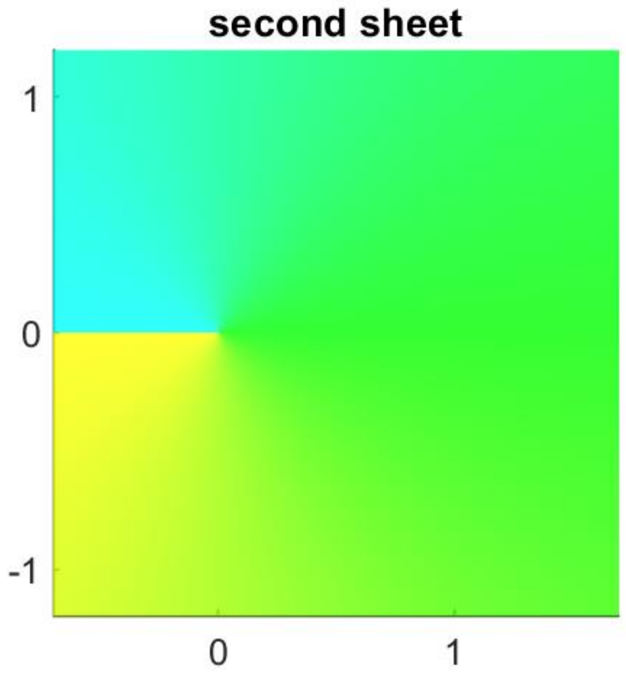
$$g(z) = c_0 + \sum_{k=1}^{n} \frac{c_k}{\log(z) - s_k}$$

Degree $n = 30$ reciprocal-log least-squares fit to $f(z) = z^{1/3}$ in 1000 clustered points on the circle $\left|z - \frac{1}{2}\right| = \frac{1}{2}$.



max error 2×10^{-9}

By adding $2\pi i$ to $\log(z)$ in the formula defining g, you get an approximation to f on the next Riemann sheet.



max error 2×10^{-6}

Reciprocal-log approximation: some questions

$$g(z) = \sum_{j=1}^{m} \sum_{k=1}^{n_j} \frac{c_{jk}}{\log(z - z_j) - s_{jk}} + p_0(z)$$

- What can be proved about these approximations on Riemann surfaces?
- “Reciprocal-log Padé approximation”: Good for extrapolation? Acceleration of convergence?
- Can a log-lightning Laplace solver outperform standard lightning solvers in practice?
- Is there a log-lightning analogue for Helmholtz problems?
- Is there a reciprocal-log analogue of the barycentric formula? Of the AAA algorithm?
- Links to Double Exponential quadrature? (Similar asymptotics and reliance on Riemann sheets)
- Once we’ve gone beyond rational functions, are other forms of interest besides reciprocal-logs?

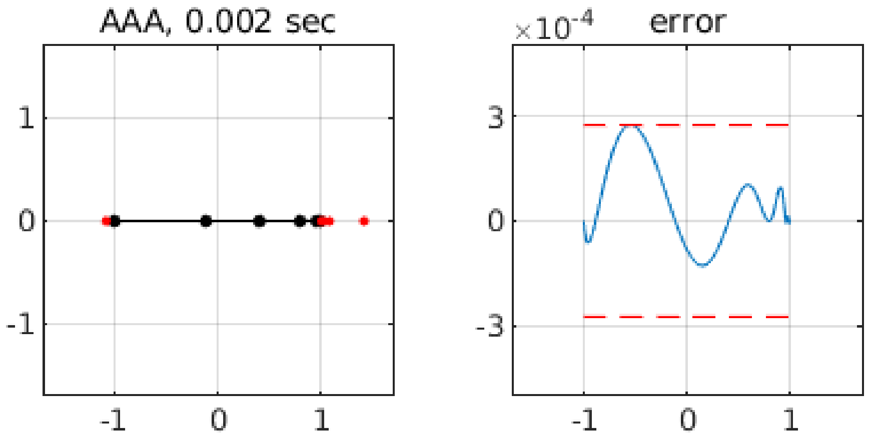
Two summary remarks

1. Rational approximations are useful for scientific computing, here and now.

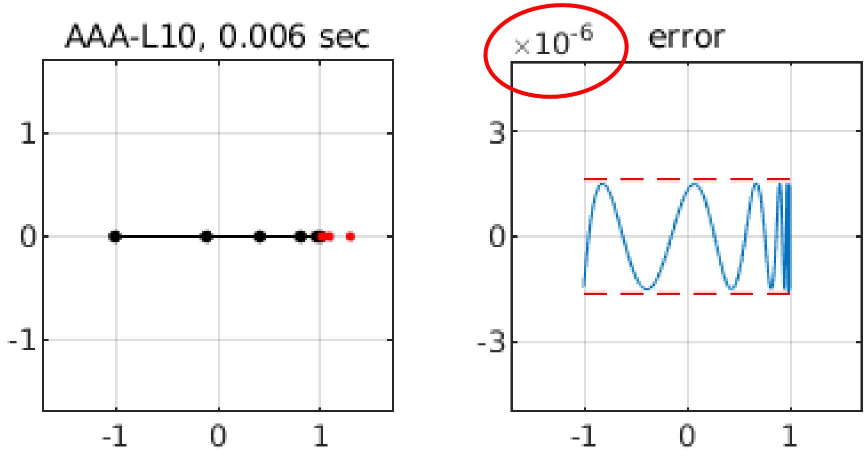
2. Reciprocal-log approximations open new possibilities for still faster PDE solvers,
   for approximations on Riemann surfaces, and perhaps in other areas too.

$\log(1.01 - x)$ on $[-1,1]$, type (6,6)

REAL APPROXIMATION



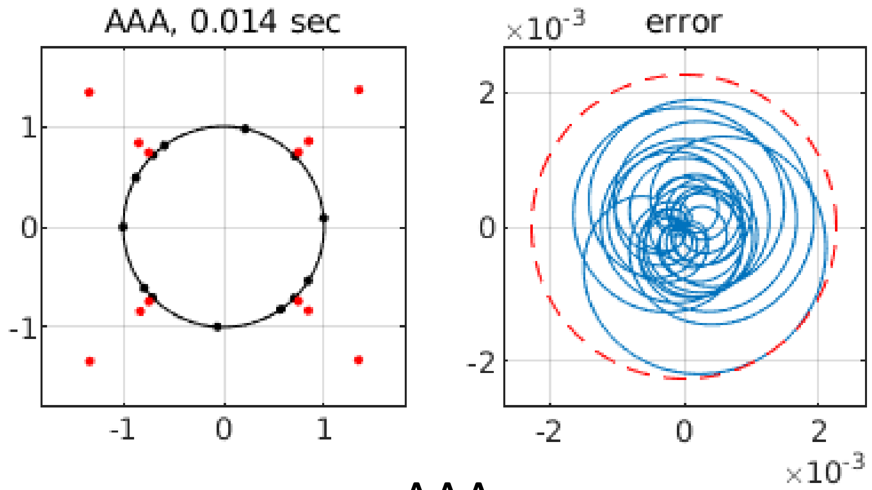
AAA



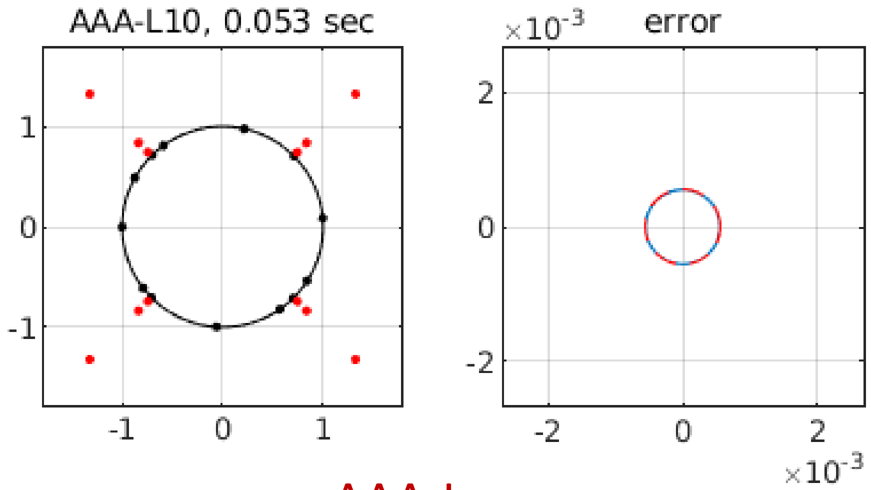
AAA-Lawson

$(1.1 + z^4)^{1/2}$ on the unit circle, type (12,12)

COMPLEX APPROXIMATION



AAA



AAA-Lawson

Tapered exponential clustering of poles

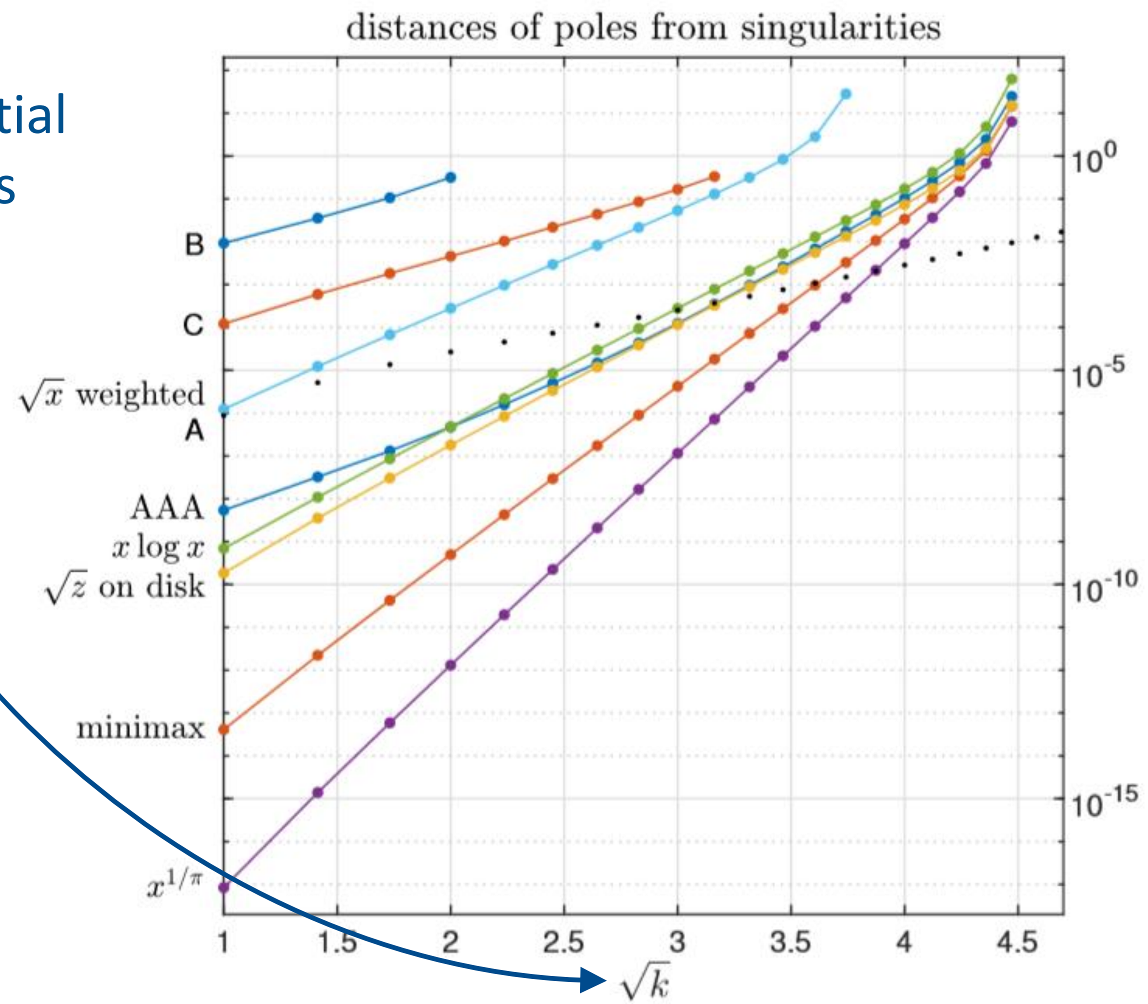


Fig. 6 Tapered exponential clustering of poles near singularities for the nine examples with free poles from Figs. 1–3 of the last section. The crucial feature is that the curves appear straight with this horizontal axis marking $\sqrt{k}$ rather than k, where $\{d_k\}$ are the sorted distances of the poles from the singularities. The data for the poles at vertex A of Fig. 3 have been deemphasized to diminish clutter (black dots), since they lie at such a different slope from the others.

An explanation of this effect via potential theory, though without theorems, is given in T.-Nakatsukasa-Weideman, *Numer. Math.* to appear.

0. A personal remark

(These are notes for me, not to be visible to viewers.)

Much of my early training was related to complex variables. I took a course In high school from the textbook by Churchill, which was taught by David Robbins. Then I wrote my undergraduate thesis at Harvard in complex approximation, and two of the readers were Birkhoff and Ahlfors. As a graduate student I was connected with Peter Henrici and I worked on Schwarz-Christoffel mapping at his suggestion.

My career as a numerical analyst since then has made constant use of complex variables. For example, the theme of my approximation theory book is that you can't understand polynomials on the unit interval without knowing about Bernstein ellipses in the complex plane. The complex plane has also been the background of a lot of my work on spectral methods for differential equations, on numerical linear algebra, and on quadrature. In the present talk, the motivation is use of complex variables for solution of PDEs.

Yet throughout my career, I have had very little contact with the complex analysis community. I know only a few of you who are listening to this talk, and over the years, when I have wanted help on this or that topic, I have generally not known who or how to ask. So I have benefited amazingly little from the expertise of people like you who know complex analysis more deeply than I do. Partly this is probably my own fault, but mainly, I think it reflects that there is not much overlap between the questions of interest to theorists and what matters in computational practice. This is disheartening for me.

Part 2 of this talk presents one of these questions. If somebody listening can help me on that one, I will be very grateful.