RATIONAL FUNCTIONS

Nick Trefethen, University of Oxford

$$r(z) = \frac{p(z)}{q(z)}$$

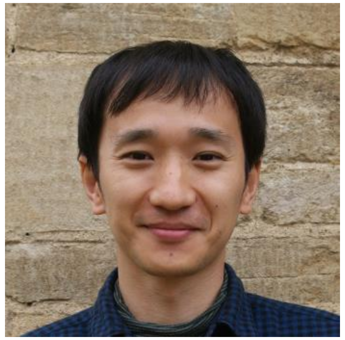
- A bit of history and philosophy
- Free poles and AAA approximation
- Fixed poles and lightning PDE solvers
- A bit more history and philosophy

Follow-on talk 2:30 this afternoon, MS37


Martin Gutknecht


Jean-Paul Berrut


André Weideman


Yuji Nakatsukasa


Olivier Sète


Laurence Halpern


Abi Gopal


Silviu Filip


Pablo Brubeck


Stefan Güttel


Bernd Beckermann


Thomas Schmelzer


Ricardo Pachón


Joris Van Deun


Elias Wegert


Anthony Austin


Wynn Tee

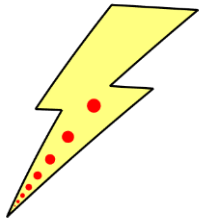

Pedro Gonnet

A bit of history and philosophy

Polynomials

poles at ∞

Rational functions



poles anywhere

Polynomials in mathematics:

- The basis of analysis (since Newton)
- The basis of complex analysis (since Weierstrass)
- The basis of algebra (forever)

Rational functions in mathematics: less fundamental.

But important for computation.

Rational functions have special powers:

- near singularities
- beyond singularities
- on unbounded domains

This talk focuses on scalars, though vectors and matrices are important too.
And everything is univariate, though multivariate is important too.

Polynomials in numerical computation (usually their presence is obvious)

interpolation and approximation	Taylor series, data fitting, splines,…
quadrature formulas	integrate a polynomial interpolant
rootfinding	`roots` and its relatives: polynomial “proxy” + eigenvalue problem
optimization	starts with Newton’s method, a degree 2 polynomial model
finite difference methods	differentiate a local polynomial interpolant
spectral methods	differentiate a global polynomial interpolant
Chebfun	continuous analogue of MATLAB

Rational functions in numerical computation (often their role is hidden)

discrete ODE formulas	linear multistep formula ⇔ rat. approx. of $\log z$ at $z = 1$
digital filters	”recursive”= “infinite impulse response”
conjugate gradients and Lanczos	Padé approximation of $u^*(zI - A)^{-1}v$
matrix eigenvalues	shifts and inversions, FEAST,…
functions of matrices	e.g., MATLAB `expm`
acceleration of convergence of series	Aitken, Shanks, Wynn, epsilon, eta,… : all based on Padé
polefinding, analytic continuation	traditionally also based on Padé
quadrature formulas	every quadrature formula ⇔ rational approximation (Gauss-Takahasi-Mori)
model order reduction, control	rational approximation + linear algebra

Polynomials

Computing with polynomials has been a problem over the years — see my "Six myths" essay. Matters have improved in the Chebfun era.

A dangerous definition: $$p(z) = \sum_{k=0}^{n} a_k z^k$$

Problem $\{z^k\}$ vary exponentially over a domain (unless it's a circle) even if $p(z)$ does not.

→ exponential ill-conditioning

Solution Use orthogonal polynomials, e.g. via Vandermonde with Arnoldi, or switch to a barycentric representation.

Rational functions

Computing with rational functions has been worse! — one reason they are not better known. Perhaps this is now beginning to improve.

A dangerous definition: $$r(z) = \frac{p(z)}{q(z)}$$

Problem p and q may vary exponentially over a domain even if r does not.

→ exponential ill-conditioning

Solution Use orthogonal bases, e.g. via rational Arnoldi, or switch to partial fractions, barycentric, or matrix pencil representations.

There has also been:

- too much minimax
- too much Padé
- too much theory

. . . at the expense of everything else

Free poles and AAA approximation

AAA (Chebfun, running in MATLAB)

```
Z = rand(2000,1) + 1i*rand(2000,1);
plot(Z,'.k','markersize',4), axis(1.5*[-1 1 -1 1]), axis square
F = sqrt(Z);
[r,pol] = aaa(F,Z);
hold on, plot(pol,'.r','markersize',10)

r(1)
r(4)
r(-4)

wegert(r)
```

```
clf
plot(Z,'.k','markersize',4), axis(1.5*[-1 1 -1 1]), axis square
F = sqrt(Z.*(1-Z));
[r,pol] = aaa(F,Z);
hold on, plot(pol,'.r','markersize',10)

wegert(r)
```

Three representations of rational functions

Quotient of polynomials

$$r(z) = p(z)/q(z)$$

Advantage: mathematically simple
Disadvantage: breaks down numerically when poles are clustered

Partial fractions

$$r(z) = \sum \frac{a_k}{z - z_k}$$

Advantages: computationally simple
easy to exclude poles from regions of analyticity
easily parallelizable
Disadvantage: leads to ill-conditioned matrices

→ lightning PDE solvers

Barycentric
(= quotient of partial fractions)

$$r(z) = \sum \frac{a_k}{z - z_k} \Big/ \sum \frac{b_k}{z - z_k}$$

Advantages: outstanding stability if $\{z_k\}$ are well chosen
decoupling of support points z_k and coefficients a_k, b_k
Disadvantage: no control over pole locations

→ AAA and AAA-Lawson

Option #4: discrete orthogonal bases à la RKFIT (Güttel) and IRKA (Gugercin et al.).
There is also the Loewner framework (Antoulas). Not in the running: continued fractions.

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Barycentric
(= quotient of partial fractions)

$$r(z) = \sum \frac{a_k}{z - z_k} \Big/ \sum \frac{b_k}{z - z_k}$$

D

Theorem. *Take any fixed distinct support points* $\{z_k\}$. *As* $\{a_k\}$ *and* $\{b_k\}$ *range over all complex values with at least one* b_k *nonzero,* r *ranges over all degree n rational functions.*

AAA algorithm (= "adaptive Antoulas-Anderson")

THE AAA ALGORITHM FOR RATIONAL APPROXIMATION

YUJI NAKATSUKASA*, OLIVIER SÈTE†, AND LLOYD N. TREFETHEN‡

For Jean-Paul Berrut, the pioneer of numerical algorithms based on rational barycentric representations, on his 65th birthday.

SISC 2018

$$r(z) = \frac{n(z)}{d(z)} = \sum_{k=1}^{m} \frac{a_k}{z - z_k} \Bigg/ \sum_{k=1}^{m} \frac{b_k}{z - z_k}$$

- Fix $a_k = f_k b_k$, so that we are in "interpolatory mode": $r(z_k) = f_k$.
- Taking $m = 1,2, \ldots$, choose support points z_m one after another.
- Next support point: sample point ζ_i where error $|f_i - r(\zeta_i)|$ is largest.
- Barycentric weights $\{b_k\}$ at each step:
  chosen to minimize linearized least-squares error $||\, fd - n \,||$.

AAA is remarkably effective, quickly producing approximations within factor ~ 10 of optimal.
The support points cluster near singularities, giving stability even in extreme cases.

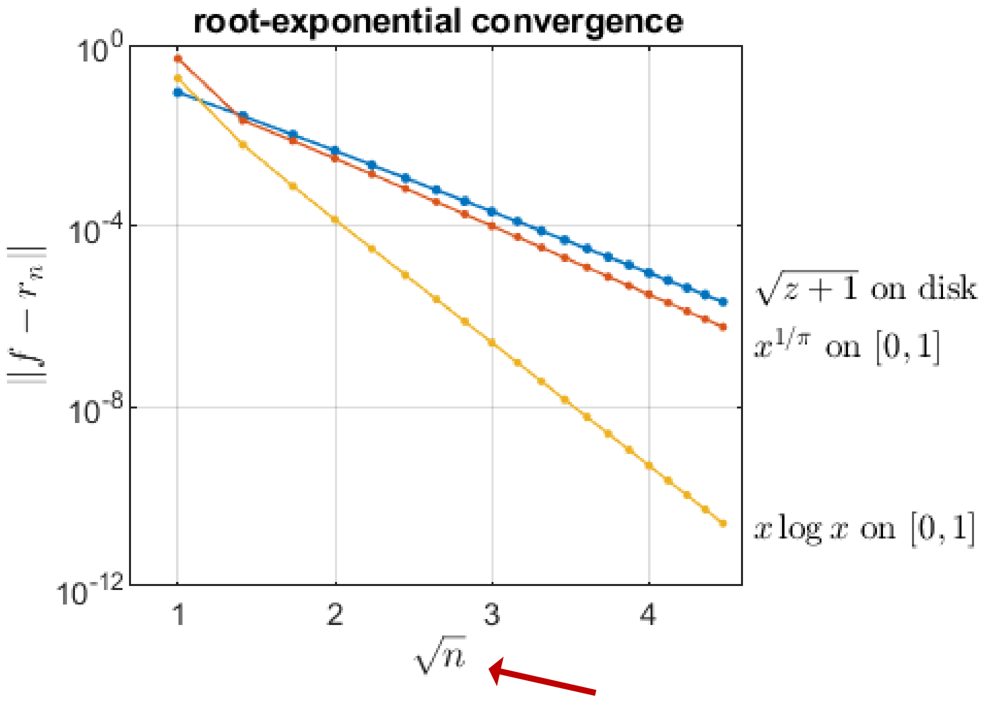
No such fast, flexible methods have existed before.
But there is no theory, and AAA sometimes fails. Big open questions here.

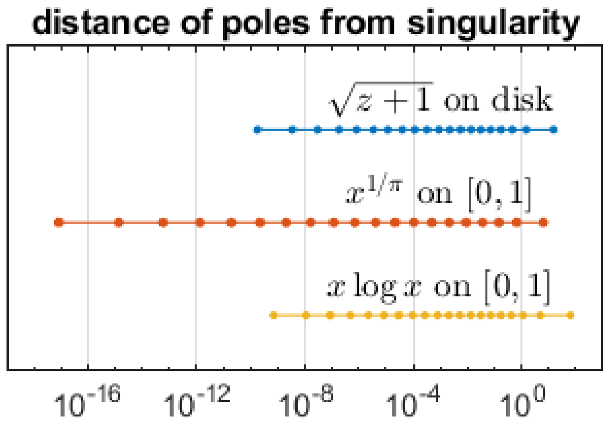
Root-exponential convergence at branch point singularities

Donald Newman 1964:

$O(\exp(-C\sqrt{n}\,))$ convergence for degree n rational best approximation of $|x|$ on $[-1,1]$
made possible by exponential clustering of poles and zeros near the singularity.

Same result holds for general branch point singularities on boundaries of domains. (Gopal & T., *SINUM* 2019)
Proof: Hermite contour integral formula… potential theory. (Walsh, Gonchar, Rakhmanov, Stahl, Saff, Totik, Aptekarev, Suetin,…)





Root-exponential convergence at branch point singularities

Donald Newman 1964:

$O(\exp(-C\sqrt{n}\,))$ convergence for degree n rational best approximation of $|x|$ on $[-1,1]$ made possible by exponential clustering of poles and zeros near the singularity.

Same result holds for general branc

Proof: Hermite contour integral forn

Hermite integral formula. *The error in degree n rational interpolation of f at points $\{x_k\}$ with poles $\{p_k\}$ is given by an integral over any contour Γ in the region of analyticity of f :*

$$f(x) - r(x) = \frac{1}{2\pi i} \int_\Gamma \frac{\phi(x)}{\phi(t)} \frac{f(t)}{t-x}\, dt,$$

where

et estimates from potential the
:harges and $\{x_k\}$ = negative cha

From here we get estimates from potential theory with $\{p_k\}$ = positive charges and $\{x_k\}$ = negative charges.

AAA approximation of conformal maps

Gopal and T., *Numerische Mathematik*, 2019

T., *Computational Methods and Function Theory*, to appear

`confmap.m` from `people.maths.ox.ac.uk/trefethen/lightning`

```
[f,finv] = confmap('L');
f(1)
finv(ans)
wegert(f)

confmap('iso');
confmap(8);
confmap(-8);
```

AAA approximation of conformal maps

Gopal and T., *Numerische Mathematik*, 2019
T., *Computational Methods and Function Theory*, to appear
`confmap.m` from `people.maths.ox.ac.uk/trefethen/lightning`

```
[f,finv] = co
f(1)
finv(ans)
wegert(f)

confmap('iso'
confmap(8);
confmap(-8);
```

Theorem (Stahl 1997 & 2012). Let f be a function analytic in the plane apart from branch points. *As $n \to \infty$, the poles of its Padé approximants converge to a set of curves connecting the branch points defined by a minimal-capacity condition.*

Fixed poles and lightning PDE solvers

The idea

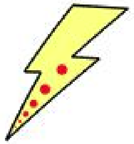
Inspired by Newman, we'd like to use AAA to solve Laplace and related PDE problems.
But AAA is only 90% reliable. Sometimes it puts poles where we don't want them.
And we don't know how to do AAA for harmonic as opposed to analytic functions.

Kirill Serkh made a suggestion (Sepember 2018).
We know poles should cluster near singularities.
Why not *fix* the poles that way, giving an easy linear approximation problem?

My last two years have been spent developing this idea.

Abi Gopal
Pablo Brubeck
Yuji Nakatsukasa
André Weideman

Lightning Laplace solver



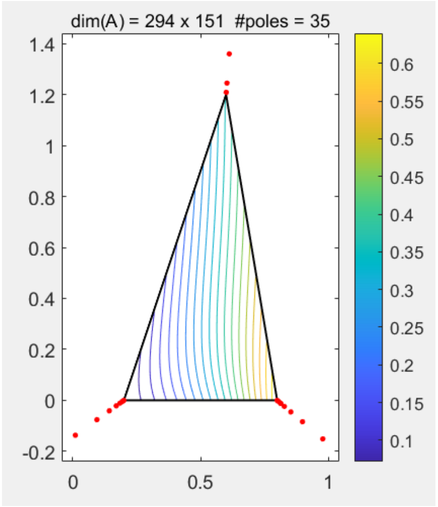
Gopal & T., *SINUM* 2019 and *PNAS* 2019
Software: `people.maths.ox.ac.uk/trefethen/`

Given: Laplace problem $\Delta u = 0$ on a 2D domain with corners.
Corner singularities are inevitable. (Wasow 1957, Lehman 1959)

Approximate $u \approx \mathrm{Re}(r)$ by matching boundary data by linear least-squares,
where r has fixed poles exponentially clustered at the corners.

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

"Newman + Runge",
a partial fractions representation



`laplace([.2 .8 .6+1.2i])`

An error bound comes from the maximum principle.
The harmonic conjugate also comes for free.

This is a variant of the Method of Fundamental Solutions, but with exponential clustering and complex poles instead of logarithmic point charges.
(Kupradze, Bogomolny, Katsurada, Karageoghis, Fairweather, Barnett & Betcke, …)

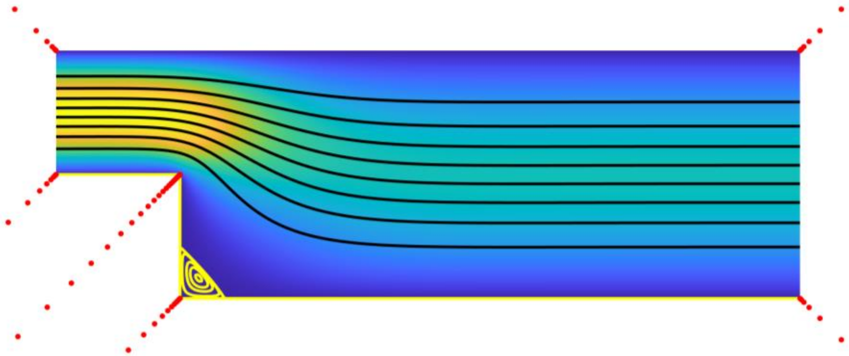
Lightning Stokes solver

(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.



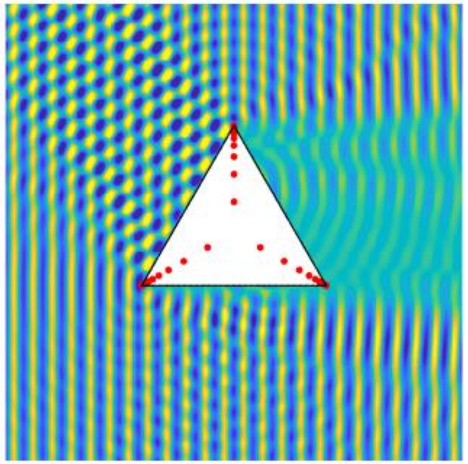
Lightning Helmholtz solver

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

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

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

Root-exponential convergence to 10 digits.



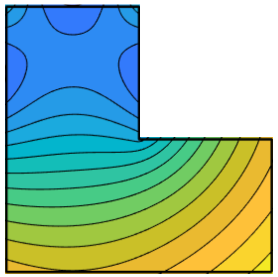
```
laplace('L');
laplace('L', 'tol', 1e-10);
laplace('iso');
laplace(12);

helm(20)
helm(-40)

stokes('step');
```

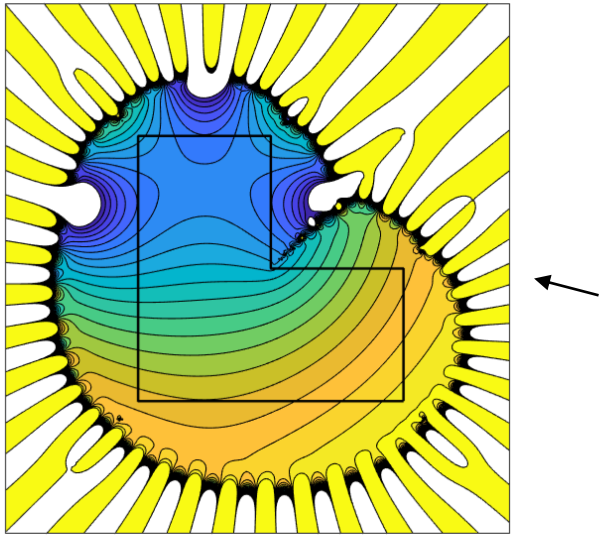
A bit more history and philosophy

Rational functions vs. integral equations for solving PDEs



Integral equation methods compute a continuous charge distribution
on the boundary, uniquely determined.
The integrals are singular, treated by clever quadrature.
The solution is evaluated by further integrals.

(Barnett, Betcke, Bremer, Bruno, Bystricky, Chandler-Wilde, Gillman, Greengard, Helsing, Hewitt, Hiptmair, Hoskins, Klöckner, Martinsson, Ojala, O'Neil, Rachh, Rokhlin, Serkh, Tornberg, Ying, Zorin,...)



Lightning methods compute a discrete charge distribution
outside the boundary, nonunique (redundant bases).
This is done by linear least-squares with no special quadrature.
The solution is evaluated as an explicit formula.

Note the branch cut, which the computation captures by a string of poles.
The yellow stripes come from the polynomial term (cf. Jentzsch's thm).

These rational approximations are prototypes of "thinking beyond the boundary." I believe we'll see more of that in the years ahead.

What is a function?

“19th century view”: singularities nowhere

Default assumption: analytic.
Use polynomials and aim for exponential convergence.

“20th century view”: singularities everywhere

Default assumption: continuous.
Real analysis is built on this, with regularity as the central concern.
Likewise much of numerical analysis (finite elements, Sobolev spaces,…).
Use piecewise polynomials. Convergence rates will be limited by regularity.

“Applied mathematics view”: singularities here and there

Default assumption: analytic except for isolated singularities.
Sometimes, we can “nail the singularities” and get exponential convergence.
More generally, use rational functions and aim for root-exponential convergence.

MS37
Nonlinear Approximation: Theory and Applications in Computational Mathematics - Part II of II

Organizer: Heather D. Wilber
Cornell University, U.S.
Anil Damle
Cornell University, U.S.

2:00 - **On Applications of Non-Linear Approximations** abstract
Gregory Beylkin, University of Colorado Boulder, U.S.

2:30 NEW - **Advanced AAA and Lightning Approximations** abstract ← Exponential clustering of poles
L. N. Trefethen, Oxford University, United Kingdom

3:00 - **Applications of Rational Function Approximation to Electronic Structure Calculations** abstract
Jonathan E. Moussa, The Molecular Sciences Institute, U.S.

3:30 - **Solving Nonlinear Eigenvalue Problems via Rational Approximation** abstract
Roel Van Beeumen, Lawrence Berkeley National Laboratory, U.S.

Closing remark