AAA-LS rational approximation and solution of Laplace problems

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Paper to appear in the proceedings, available at my website
Three representations for rational approximation on a domain $\Omega$

**Quotient of polynomials**

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

- **Advantage**: mathematically simple
- **Disadvantage**: numerical failure when poles are clustered

**Partial fractions**

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

- **Advantages**: computationally simple
  - easy to work with the real part (harmonic)
  - easy to exclude poles from $\Omega$
- **Disadvantage**: where do we put the poles?

**Barycentric**

(= quotient of partial fractions)

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

- **Advantages**: outstanding numerics if $\{z_k\}$ are well chosen
  - decoupling of support pts $z_k$ and coeffs $a_k, b_k$
- **Disadvantage**: no way to exclude poles from $\Omega$

→ **lightning PDE solvers (2019)**

→ **AAA rational approximation (2018)**
1. Free poles and AAA approximation
AAA  (Chebfun, running in MATLAB)

\[
Z = \text{rand}(2000,1) + 1i \times \text{rand}(2000,1);
\]
\[
\text{plot}(Z,'.k','markersize',4), \text{axis}([-1 2 -1.5 1.5]), \text{axis square}
\]
\[
F = \sqrt{Z \times (1-Z)};
\]
\[
\text{tic, [r,pol] = aaa(F,Z); toc}
\]
\[
\text{hold on, plot(pol,'.r','markersize',10)}
\]
\[
\text{norm(F-r(Z),inf)}
\]
\[
\text{phaseplot(r)}
\]
AAA algorithm (= “adaptive Antoulas-Anderson”)

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

- 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 \(\zeta_i\) 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.
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,...)

These data are for best approximations. AAA would be similar but noisier.
2. 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 we don’t know how to do AAA for harmonic as opposed to analytic functions.

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

Much of my last three years have been spent developing this idea.

Abi Gopal
Pablo Brubeck
Yuji Nakatsukasa
André Weideman
Stefano Costa
Peter Baddoo
Given: Laplace problem $\Delta u = 0$ on a 2D domain with corners. Corner singularities are inevitable. (Wasow 1957, Lehman 1959)

Approximate $u \approx \text{Re}(r)$ 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 plus a polynomial term

An error bound comes from the maximum principle.
The harmonic conjugate also comes for free: Hilbert transform or Dirichlet-to-Neumann map.

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, Karageorghis, Fairweather, Barnett & Betcke, ...)

Software: people.maths.ox.ac.uk/trefethen/

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

**Lightning Stokes solver**

(Brubeck & T., *SISC*, submitted)

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

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

Root-exponential convergence to 10 digits.
Lightning Stokes solver — triangular lid-driven cavity

Fig. 5.4. Stokes flow in a triangular lid-driven cavity of vertex angle $2\alpha = 28.5^\circ$. There are 49 poles at each corner, of which 7 at the lower corner and 5 at each upper corner lie outside the plotting axes. The computed result matches Taneda’s experiment from 1979 [35].
laplace('L');
laplace('L', 'tol', 1e-10);
laplace('iso');
laplace(12);

helm(20)

helm(-40)

stokes
3. New algorithm: AAA-LS

= Adaptive Antoulas-Anderson—Least-Squares
Laplace problem: given $\Omega$ and real bdry data $h$, find $u$ s.t. $\Delta u = 0$ in $\Omega$ and $u = h$ on $\partial \Omega$.

AAA-LS finds a complex rational function $r$ s.t. $|f - r| < \varepsilon$ on $\partial \Omega$, discards poles in $\overline{\Omega}$, then computes a least-squares fit to $u \approx h$ by real parts of the remaining poles.

**AAA-LS LAPLACE SOLVER**

1. Run AAA to get rational approx $r \approx h$ with poles both in and outside $\Omega$.
2. Discard poles in $\overline{\Omega}$.
3. Solve $Ax \approx b$ to construct a new fit involving just the poles outside $\overline{\Omega}$.

Core code, given column vectors $Z$, $H$ of sample pts and data, row vector $\text{pol}$ of poles.

```plaintext
\begin{align*}
d &= \min(\text{abs}(Z-\text{pol}),[],1); & \text{for column normalization} \\
P &= Z.^(0:n); Q = d./(Z-\text{pol}); & \text{polynomial & rational columns} \\
A &= [\text{real}(P) \text{ real}(Q) -\text{imag}(P) -\text{imag}(Q)]; & \text{fitting matrix} \\
c &= \text{reshape}(A\backslash H,[],2)*[1;1i]; & \text{least-squares solve}
\end{align*}
```

**FASTER “LOCAL AAA-LS” VARIANT**

(1′) Use separate AAA fits near different corners or other singularities.
AAA-LS example: smooth domain

From a Laplace solver it’s an easy step to conformal mapping.

global variant
46 poles inside, discarded.
30 poles outside, retained.
9-digit accuracy in 0.7 secs.
AAA-LS example: L-shaped domain

global variant
12 secs. (global AAA, 294 poles)

local variant
0.7 secs. (6 local AAA fits)

NA Digest test value
\( u(0.99 + 0.99i) \approx 1.0267919261 \) accurate to 10 digits.
AAA-LS example: domain with curved sides

No new issues arise with this problem. These methods converge root-exponentially so long as the boundary is piecewise analytic.
AAA-LS example: doubly connected domain

To treat the hole, we include polynomials in both $(z - z_c)^{-1}$ and $z$.  (Runge 1865)
We also include a term $\log|z - z_c|$.  (Walsh 1929.  See Axler in *MAA Monthly* 1986,  
"Harmonic functions from a complex analysis viewpoint").
AAA-LS example: exterior domain, triply connected

Now there are polynomials in three reciprocals \((z - z_j)^{-1}\), but no polynomial in \(z\). Also three log terms \(\log|z - z_j|\).
AAA-LS example: real zigzag function

Zigzag function on \([-1,1]\)

Poles of local AAA approximants

Error in AAA-LS rational approximant

local variant

466 finite poles.
962 total degrees of freedom.
2 poles in \([-1,1]\) are discarded.
7-digit accuracy in 0.7 secs.
AAA-LS for computing the Hilbert transform on the real line

Hilbert transform ≈ principal value integral ≈ harmonic conjugate ≈ Dirichlet-to-Neumann map. Comes for free from any rational approximation of a real function $u$.

Prototype code

```matlab
function [v,f] = ht(u)
X = logspace(-10,10,300)'; X = [X; -X];
 [~,pol] = aaa(u(X),X,'cleanup',0);
 pol(imag(pol)>=-0) = []; pol = pol.';
 d = min(abs(X-pol),[],1);
 A = d./(X-pol); A = [real(A) -imag(A)];
 c = reshape(A\u(X),[],2)*[1;1i];
 f = @(x) reshape((d./(x(:)-pol))\c,2); size(x));
 v = @(x) imag(f(x));
```

This plot was produced in 2 secs.
AAA-LS theory

Laplace problem: given $\Omega$ and real bndry data $h$, find $u$ s.t. $\Delta u = 0$ in $\Omega$ and $u = h$ on $\partial \Omega$.

AAA-LS (the global variant) finds a complex rational function $r$ s.t. $|f - r| < \varepsilon$ on $\partial \Omega$, discards poles in $\bar{\Omega}$, and computes a least-squares fit to $h$ by real parts of the remaining poles.

**Theorem.** If $\Omega$ is a disk or half-plane, this method gives accuracy $< 2\varepsilon$.

For a precise statement and proof, see the paper.

If $\Omega$ is not a disk or half-plane, examples show that the method can fail, but it appears such examples are nongeneric. Further investigation needed.
Integral equations vs. rational functions 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.


AAA/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 by an explicit formula.

Note the branch cut, which the computation captures by a string of poles. The yellow stripes come from the polynomial “Runge” 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. With luck, maybe even in 3D.
In closing: what is a function?

“18th 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.
Not mentioned in this talk: “log-lightning” approximations with near-exponential convergence.
(Nakatsukasa & T., SINUM, submitted; Baddoo & T., in preparation)