Spurious Poles

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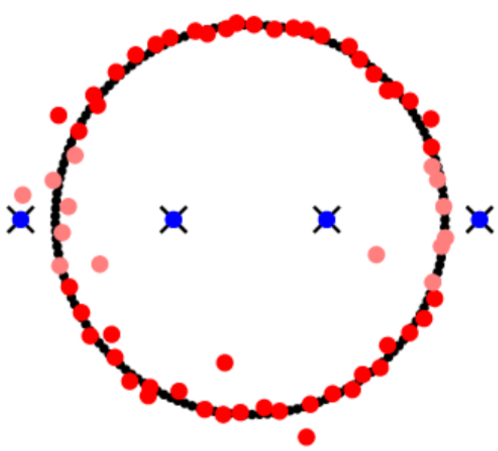


Outline:

discussion - - > new algorithm

Thanks to Stefano Costa

Rational approximation

Problem

Given information about a function f in the complex plane,
find a rational function r that in some sense approximates f.

Approximation theory motivation

Rational functions are much more powerful than polynomials if

- f has singularities in or near the domain of interest, or
- The domain is large or unbounded

Applications motivation

Evaluation of $f(z)$ on computers is less interesting than

- Model order reduction
- Evaluation of $f(A)$ where A is a matrix or operator
- Numerical solution of PDEs (my talk on Friday)
- Identification of poles; analytic continuation
- Other indirect uses of rational approximations

this minisymposium

For simplicity I'll speak as if all poles are simple and finite.
Degree n means $\leq n$ poles.

Spurious poles / Froissart doublets

pole with residue ≈ 0	$\approx$	nearly coincident pole-zero pair

...with no apparent analytic connection to f.

These can appear in theory (exact arithmetic),
and they invariably appear when there is rounding error or other noise.
Some say "Froissart doublet" only in the latter case, but I will not distinguish.

Spurious poles cause lots of trouble, both theoretical and computational.

Note that their influence is highly localized.
Further away, their effect on $r(z)$ is very small.

Spurious poles in Padé approximation: theory

Padé: choose r to match the first $2n+1$ terms of the Taylor series of f.

Dumas (1908) and Perron (1913): spurious poles may
prevent pointwise convergence as $n \to \infty$.

Wallin (1972): one may even get divergence $\forall z \neq 0$, and even when f is entire.

Nuttall-Pommerenke theorem (1973): *convergence in capacity*.
As $n \to \infty$, spurious poles need not go away, but they get weaker.

Stahl (1997): generalization to f with branch points.

Gonchar, Rakhmanov, Aptekarev, Suetin, Saff, Lubinsky...: further generalizations
including to multipoint Padé and Padé-Hermite approximation.

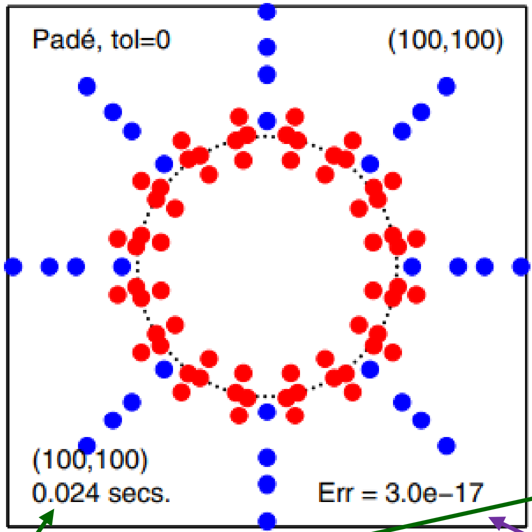
Despite this difficult theoretical situation, spurious poles
are in practice not so common in exact arithmetic.
But with rounding errors or other noise, they are everywhere.

Spurious poles in Padé approximation: computation

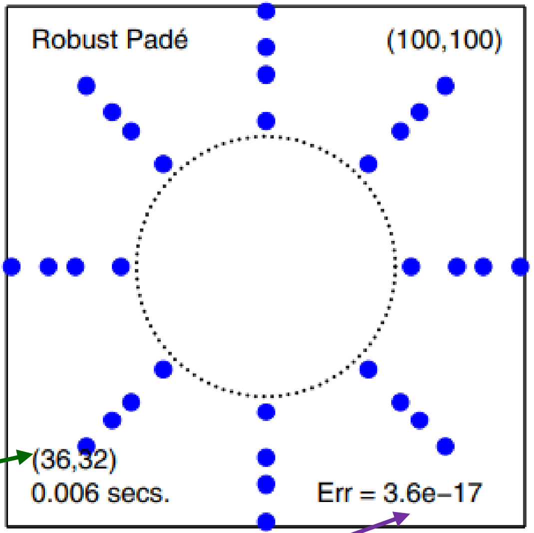
From Gonnet-Güttel-T., “Robust Pade approximation via SVD”, *SIREV* 2013.
Type (100,100) Padé approximation of $\tan(z^4)$.

Red dots mark poles with residue $< 10^{-12}$.

Straight Padé



Padé with SVD regularization



Degree reduces from 100 to 36.

Error increases very little.
(Depends on what you measure. Error = ∞ at poles.)

Chebfun: see `padeapprox` and `ratinterp`

Padé approximation and best approximation get too much attention!

Most rational approximation theory literature concerns these two problems.
Note that both are defined by exact optimality (at a point; over a domain).

Exact optimality leads to pathologies in certain situations.
There are hundreds of papers analysing these pathologies.

But who says our approximations need to be Padé or best?
Users of rational approximations should focus on more robust formulations.

Rational approximation belongs to analysis, not algebra.

ANALOGY: MATRIX ITERATIONS

To solve $Ax = b$ iteratively, we seek $x_1, x_2, \ldots$ such that $x_k \to x$ fast.
All kinds of preconditioners come into play.
We do not aim for x_k to be exactly optimal in any sense.

Imagine if 200 papers had been published on "Lanczos theory" and only 20 on actually solving $Ax = b$.

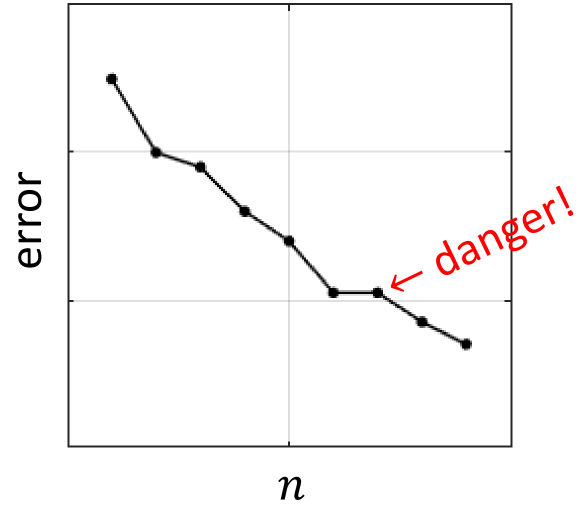
Intuition about spurious poles

Since a spurious pole is localized, it confers little benefit on an approximation.

So if r_n has a spurious pole, $\exists r_{n-1}$ that is nearly as good.
...provided we define “nearly as good” as analysts, not algebraists.

In Padé approximation, for example:
r_n might match 10 Taylor coeffs of f exactly, with a spurious pole;
r_{n-1} might match the same coeffs to accuracy 10^{-10}, with no spurious pole.

So spurious poles tend to appear where convergence is stagnating.
This will happen almost invariably when there is noise.



A theorem confirming this intuition

A pole can lie hidden in an approximation domain, but only if it is very weak.

Theorem. *Suppose f is analytic for $|z| \le 1$ and $|f(z) - r(z)| \le \varepsilon$ for $|z| = 1$, where r is a rational function with just a simple pole in the unit disk at $z = a$. Then the residue of r at $z = a$ is $< 2\varepsilon$ in absolute value.*

Proof. Write $r(z) = g(z)/(z - a)$ and consider $f(z)(z - a) - g(z)$.
It is analytic for $|z| \le 1$ and $\le \varepsilon(1 + |a|) < 2\varepsilon$ for $|z| = 1$. So $|g(a)| < 2\varepsilon$ by the maximum modulus principle, and $g(a)$ is the residue of r at $z = a$.

QED.

AAA algorithm

"Adaptive Antoulas-Anderson", using barycentric representation.
Nakatsukasa, Sète & T., *SISC* 2018.
Fast computation of near-best approximations on arbitrary domains,
typically represented by thousands of points on the boundary.
No theory, but outstanding practice.

Standard implementation: Chebfun `aaa`

Often, no trouble with spurious poles.
They tend to arise, however, if:

- The accuracy is close to machine precision
- Other noise is present
- A boundary is underresolved, especially near singularities
- A real function is being approximated on a real interval

By default AAA applies a "cleanup" procedure that often helps.

AAA examples

```
Z = exp(2i*pi*(1:100)'/100);
F = tan(Z);
tic, [r,pol] = aaa(F,Z); toc
length(pol)
norm(F-r(Z),inf)
plot(Z,'.k'), axis equal, hold on, grid on
plot(pol,'.r','markersize',12), hold off
pol
pi/2
```

cloud

square

interval

New algorithm with no spurious poles: AAA-LS

Stefano Costa and I have developed a new algorithm.
Paper to appear in the proceedings of this conference (see my website):

"AAA-least squares rational approximation and solution of Laplace problems"

For the Laplace problems, see my talk on Friday.

AAA-LS ALGORITHM

(1) Run AAA to get an approximation that may have some bad poles.
(2) Discard the bad poles.
(3) Solve $Ax \approx b$ to construct a new fit involving just the good poles.

Step (1) is in barycentric representation; step (3) is in partial fractions.

One can prove this is accurate on a disk or a half-plane.

FASTER "LOCAL AAA-LS" VARIANT

(1') Use separate AAA fits near different corners or other singularities.

AAA-LS examples

```
type aaaLS
```

$\boxed{\texttt{cloudLS}}$

$\boxed{\texttt{squareLS}}$

$\boxed{\texttt{intervalLS}}$

$\boxed{\texttt{zigzag}}$