Robust Padé Approximation

Nick Trefethen, Oxford University

HAPPY BIRTHDAY
CLAUDE + SEBASTIANO !

Robust Padé Approximation

Nick Trefethen, Oxford University

with

Pedro Gonnet

Stefan Güttel

a follow-on of earlier work on rational interpolation in roots of unity and Chebyshev points with

Ricardo Pachón

Joris van Deun

Pachón, Gonnet & van Deun, Fast and stable rational interpolation in roots of unity and Chebyshev points, in revision for *SINUM*.

Gonnet, Pachón & T, Robust rational interpolation and least-squares, *ETNA* 2011

Gonnet, Güttel & T, Robust Padé approximation via SVD, in preparation.

THE POWER OF RATIONAL INTERPOLANTS

P_m = {polynomials of degree at most m} $p_m(z)$

R_{mn} = {rational functions of type (m,n)} $r_{mn}(z) = p_m(z)/q_n(z)$

Rational interpolation: $r_{mn}(z_k) = f(z_k)$, $0 \le k \le m+n$ (generically)

Padé approximation: $f(z) - r_{mn}(z) = O(z^{m+n+1})$ (generically)

APPLICATIONS

• Extrapolation of sequences/series	Aitken, Shanks, epsilon, eta, ...
• Analytic continuation, finding poles	Padé, Chebyshev-Padé,...
• QR and other matrix iterations	shift & invert, rational Krylov,...
• Digital filters	"IIR" approxs for low-pass, high-pass,...
• Stiff ODEs & PDEs	every implicit formula uses a ratl approx
• Exponential integrators	exploiting a global approx of exp(z)
• Inverse Laplace transform	exploiting quadrature $\leftrightarrow$ ratl approx link
• Model reduction, optimal control	approx on the imaginary axis
• Exponential of a matrix	e.g. Padé (13,13) for Matlab's expm
• Pseudodifferential operators	one-way wave eqs., absorbing BCs,...
• Adaptive spectral methods	fronts, boundary layers, blow-up,...

THE FRAGILITY OF RATIONAL INTERPOLANTS

- Sometimes they do not exist or are nonunique.
- Often ill-conditioned or ill-posed. Spurious pole-zero pairs are a problem.
- Much of the available theory seems a long way from numerical practice.
- It's a rare application that dares to compute a rational approximation on the fly.

Example of nonexistence: there is no $r \in R_{11}$ s.t. $r(0)=1$, $r'(0)=0$, $r''(0)=1$.

Example of ill-posedness:

Pole-zero pair or "Froissart doublet" – D. Bessis, Friday 9:00

Type (1,1) Padé for $1+x^2$: 1

Type (1,1) Padé for $1+\varepsilon x+x^2$: $(1-(1-\varepsilon^2)x/\varepsilon) \,/\, (1-x/\varepsilon)$

POLE: $x = \varepsilon$
ZERO: $x = \varepsilon/(1-\varepsilon^2)$

Example of awkward theory: theorems on convergence of Padé approximants only assert convergence in capacity or measure, not pointwise.

OUR PHILOSOPHY: derive approximations without pole-zero doublets via robust linear algebra / regularization, using SVD

LINEAR ALGEBRA

Our strategy: work with the singular values $\sigma_1, \ldots, \sigma_n$ of the rectangular matrix C

Given $f = c_0 + c_1 z + c_2 z^2 + \ldots$, $m \geq 0$, $n \geq 0$.

$$\mathbf{a} = \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_m \end{pmatrix}, \qquad \mathbf{b} = \begin{pmatrix} b_0 \\ b_1 \\ \vdots \\ b_n \end{pmatrix}, \qquad p(z) = \sum_{k=0}^{m} a_k z^k, \qquad q(z) = \sum_{k=0}^{n} b_k z^k.$$

$$\begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \\ \vdots \\ a_m \\ \hline a_{m+1} \\ \vdots \\ a_{m+n} \end{pmatrix} = \begin{pmatrix} c_0 & & & \\ c_1 & c_0 & & \\ \vdots & & \ddots & \\ c_n & c_{n-1} & \cdots & c_0 \\ \vdots & \vdots & & \vdots \\ c_m & c_{m-1} & \cdots & c_{m-n} \\ \hline c_{m+1} & c_m & \cdots & c_{m+1-n} \\ \vdots & \vdots & \ddots & \vdots \\ c_{m+n} & c_{m+n-1} & \cdots & c_m \end{pmatrix} \begin{pmatrix} b_0 \\ b_1 \\ \vdots \\ b_n \end{pmatrix}$$

must be 0

must be a null vector of C

n x (n+1) matrix C

Trouble comes if C has rank <n, or numerical rank < n

BLOCK STRUCTURE IN THE PADÉ TABLE

The Padé table is the array of all Padé approximants to a fixed function f:

$$\begin{pmatrix} r_{00} & r_{10} & r_{20} & \cdots \\ r_{01} & r_{11} & r_{21} & \cdots \\ r_{02} & r_{12} & r_{22} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

Each Padé approx r (≠0) fills some (k+1)x(k+1) square block of the table:

$$\begin{pmatrix} r_{\mu\nu} & \cdots & r_{\mu+k,\nu} \\ \vdots & & \vdots \\ r_{\mu,\nu+k} & \cdots & r_{\mu+k,\nu+k} \end{pmatrix}$$

Our computational goals:

(1) Always return the upper-left entry $r_{\mu\nu}$, i.e. in lowest terms

(2) Achieve this not only in exact arithmetic, but to some reasonable approximation also when there are errors e.g. from rounding

SINGULAR VALUES AND POSITION IN THE BLOCK

The rank deficiency of C follows this pattern in a square block:

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 2 & 2 & 1 & 0 \\ 0 & 1 & 2 & 2 & 1 & 0 \\ 0 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

So you can tell if you're inside a square block from the singular values.
You can tell the bottom row/right column from leading zeros of a and b.
You can tell the top row/left column from trailing zeros of a and b.

From such observations we get:

THEOREM. *The following algorithm is guaranteed to converge in exact arithmetic, and takes at most* $3+\log_2$(*blocksize*) *steps*.

ALGORITHM BASED ON SVD

1. If $n=0$, set $a_0,\ldots,a_m$ equal to $c_0,\ldots,c_m$ and $b_0=1$ and go to Step 3.

2a. Compute the SVD of C and set $\rho=\text{rank}(C)$. If $\rho=n$, get q from the null singular vector b of C and then p from the matrix equations.
If $b_0 = \ldots = b_{\lambda-1} = 0$ for some $\lambda\geq 1$, which implies also $a_0 = \ldots = a_{\lambda-1} = 0$, cancel the common factor z^{λ} in p and q.

2b. If $\rho < n$, reduce n to ρ and m to $m-(n-\rho)$ (or to 0 if $r=0$) and return to Step 1.

3. Remove trailing zero coefficients, if any, from $p(z)$ or $q(z)$.

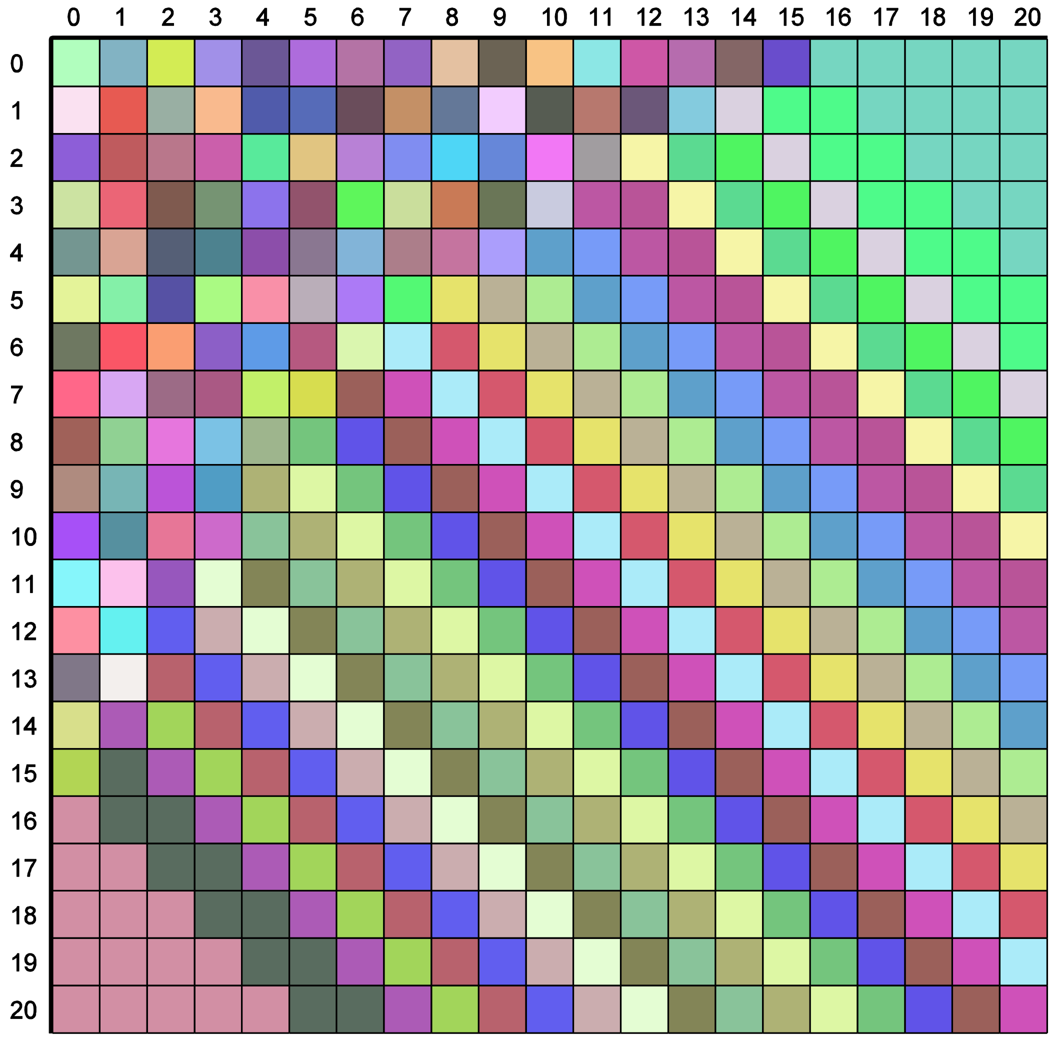
ROBUST ALGORITHM FOR PROBLEMS WITH ROUNDING ERRORS OR OTHER NOISE

The same, but with decisions about rank and zeros based on a finite tolerance.

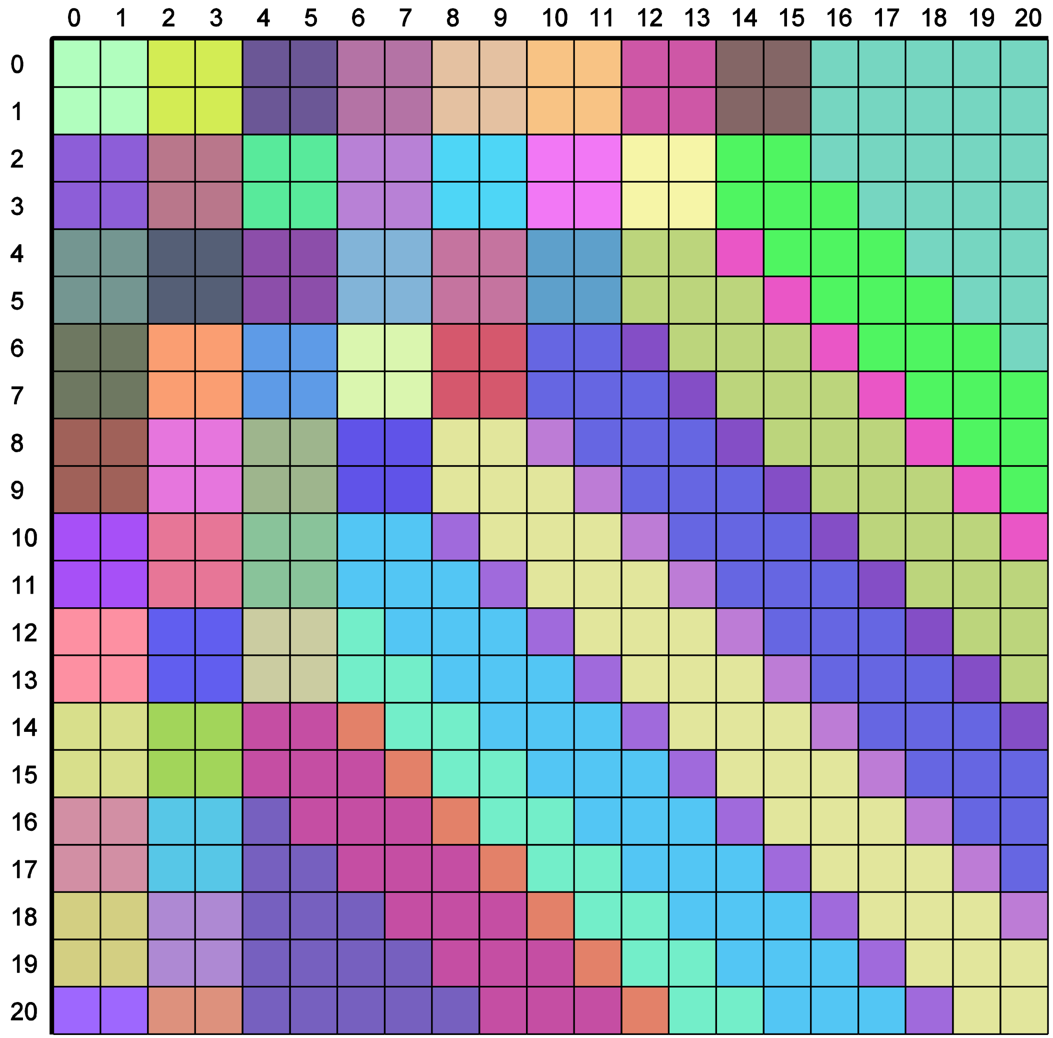
DEMONSTRATION: PADÉ TABLES

`table` `table2`

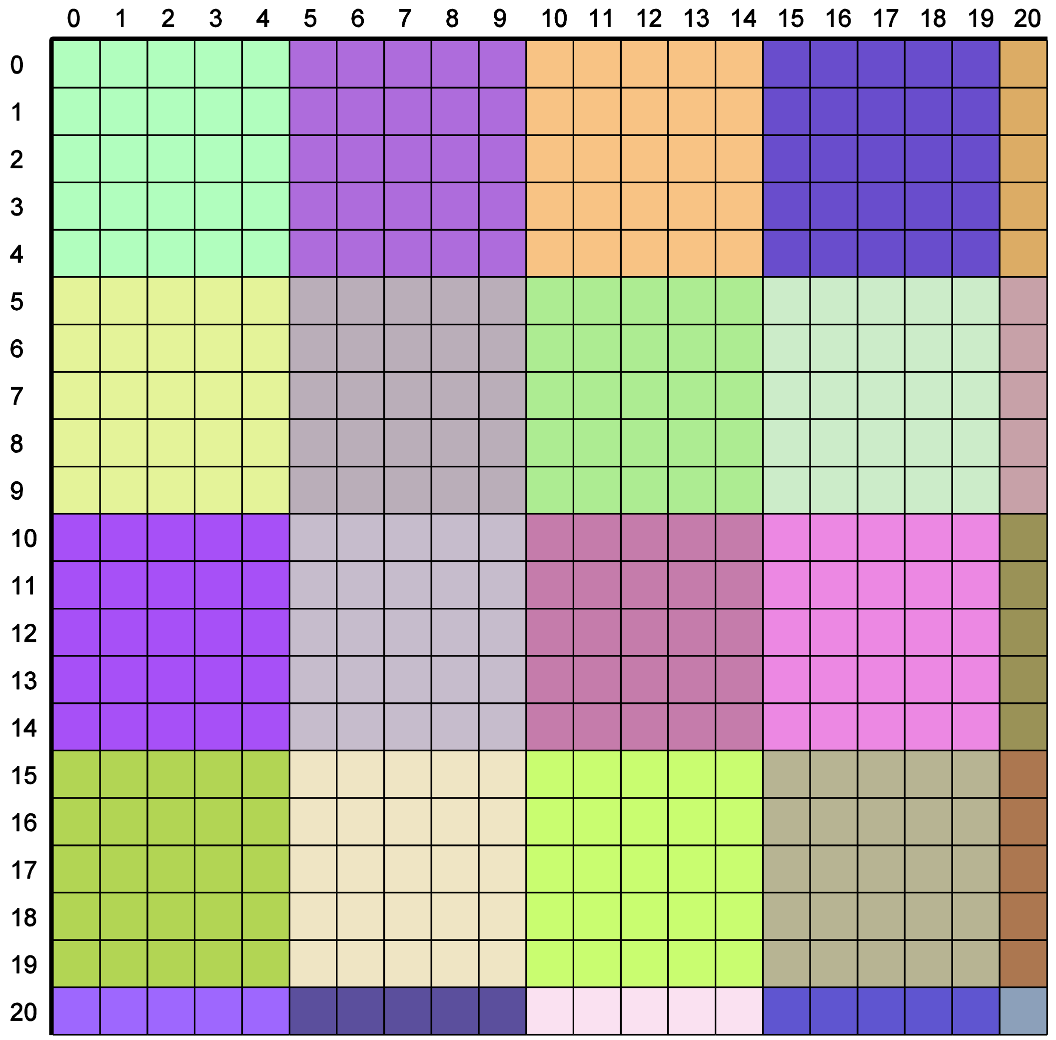
exp(z)


0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

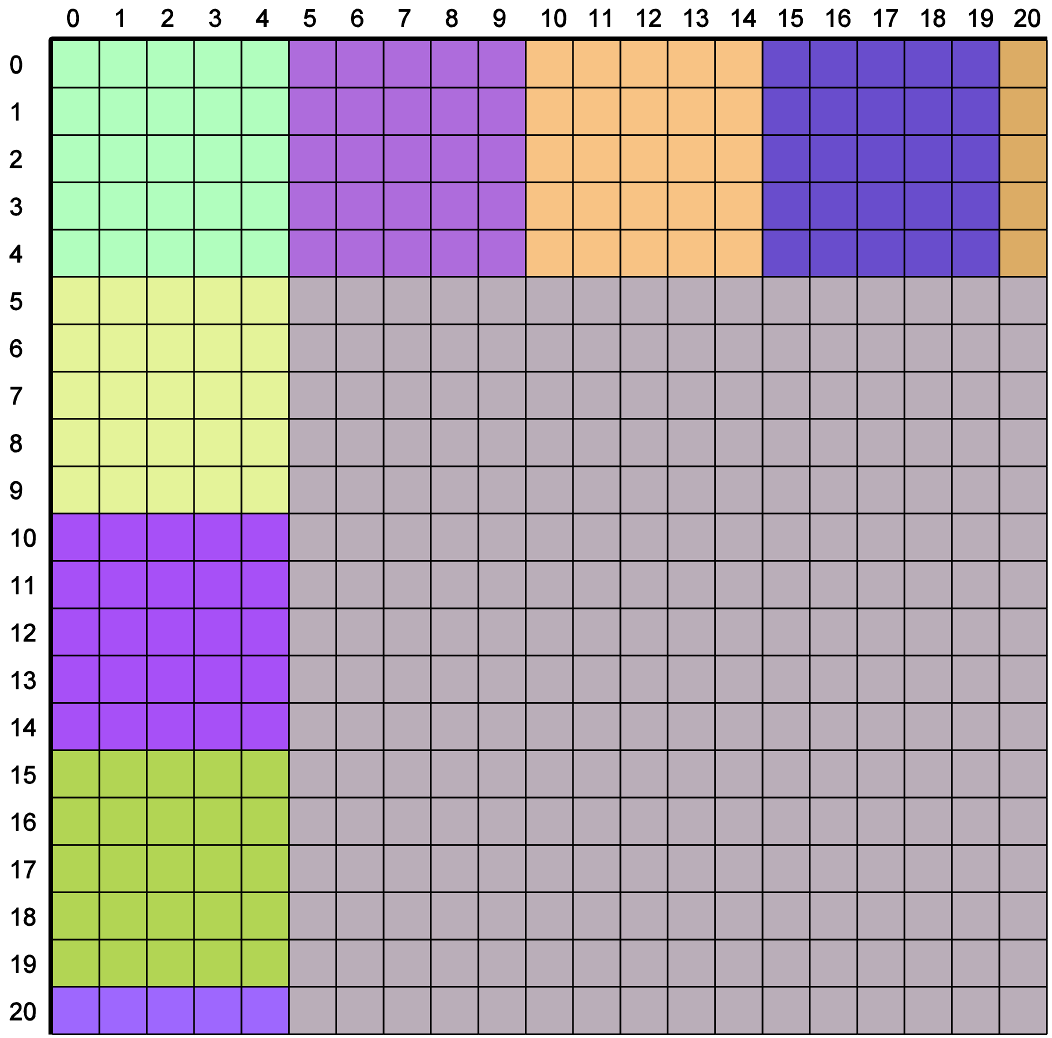
cos(z)


0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

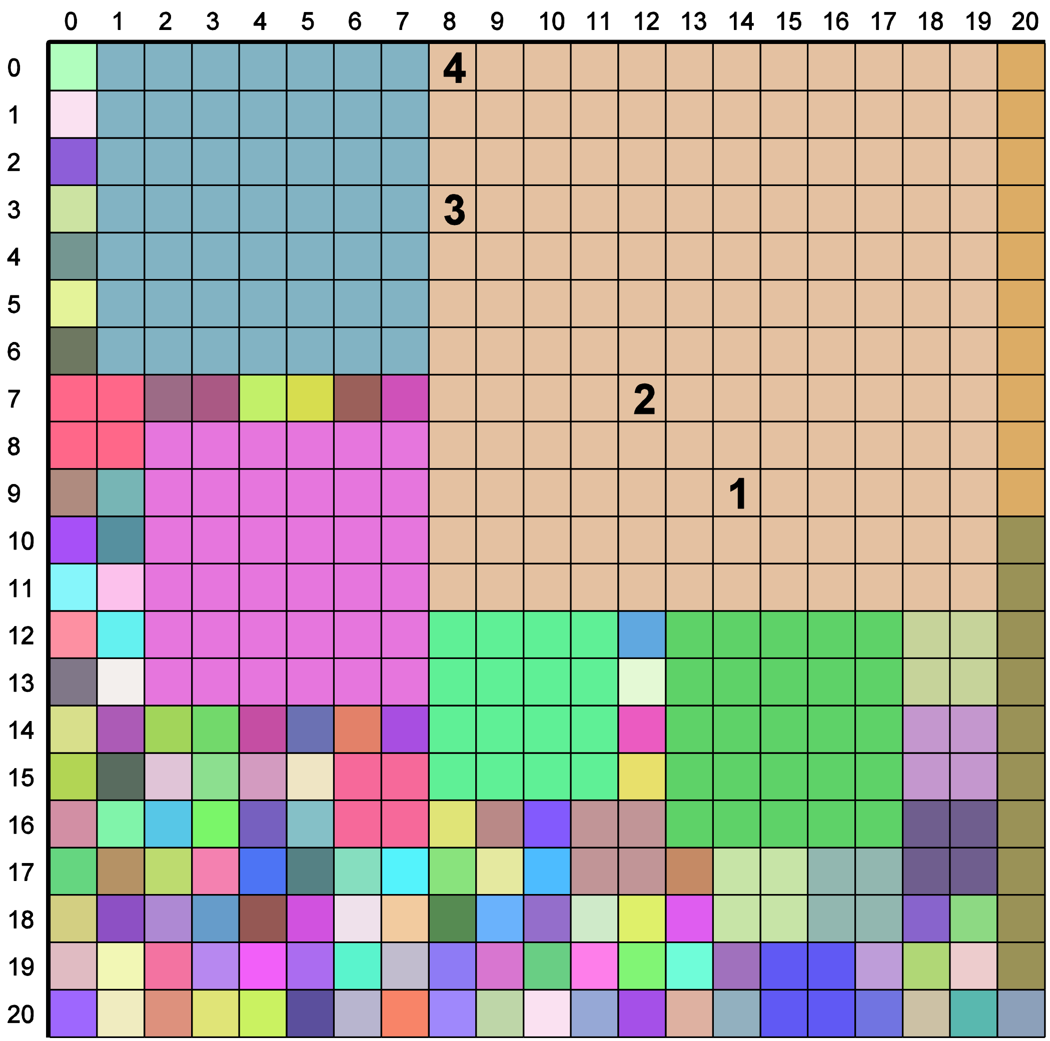
$\log(5+z^5)$


0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

$(z^5-1) / (z^5+1)$


0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

$$1 + z + z^8 + z^{20} + z^{30}$$



0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
4
3
2
1

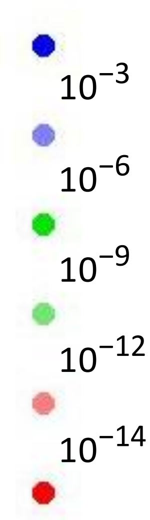
DEMONSTRATION: COMPUTED POLES

`dots`

Left: non-robust algorithm (tol=0)

Right: robust algorithm (tol=10^{-14})

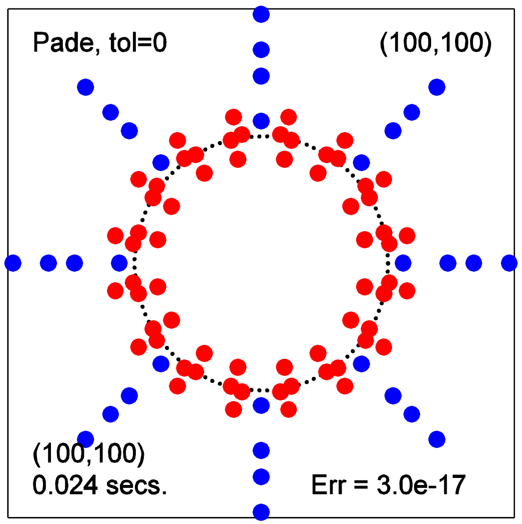
Dots show poles of r, color-coded to indicate the size of the residue:

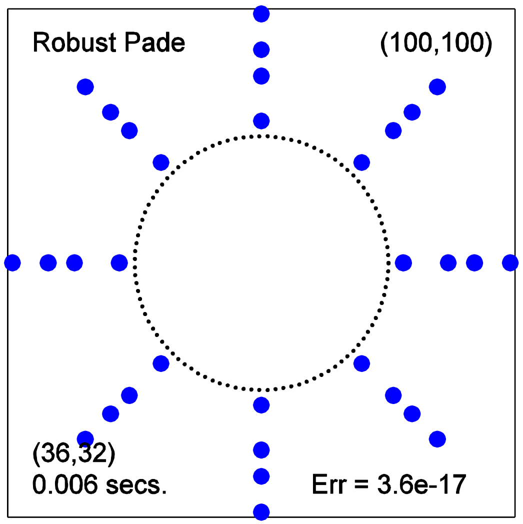


← probably genuine

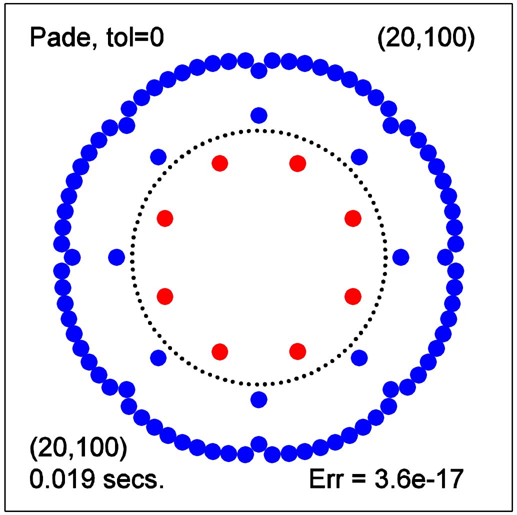
← probably spurious

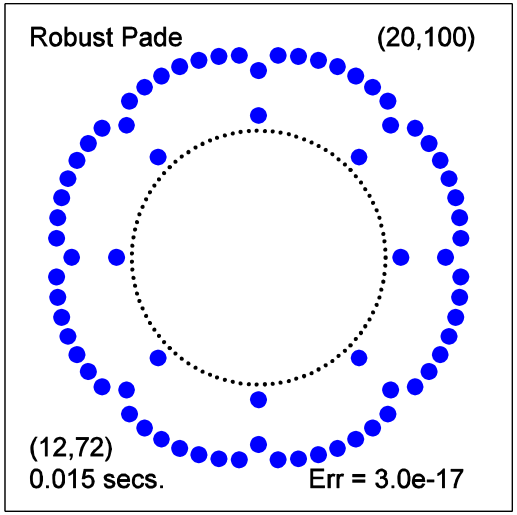
$\tan(z^4)$, type (100,100)



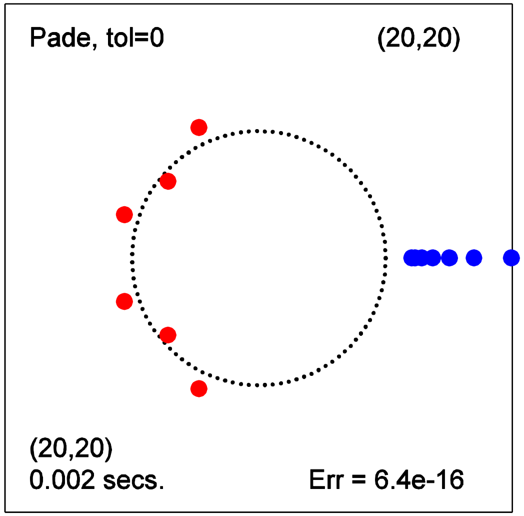


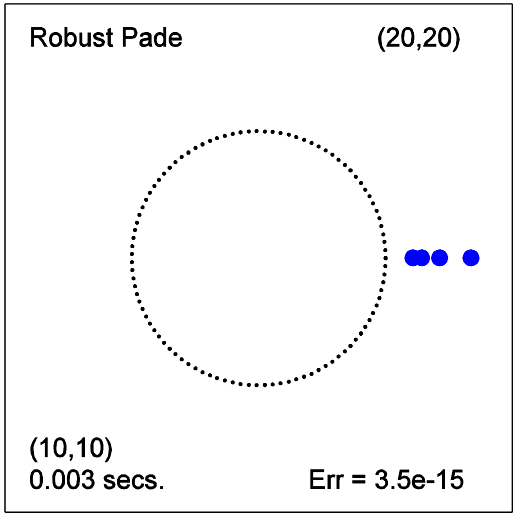
$\tan(z^4)$, type (20,100)



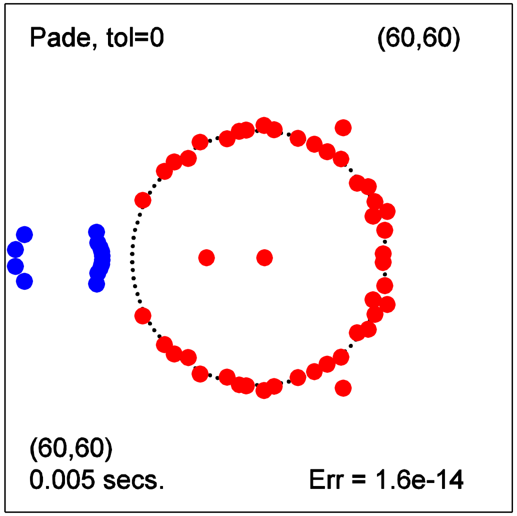


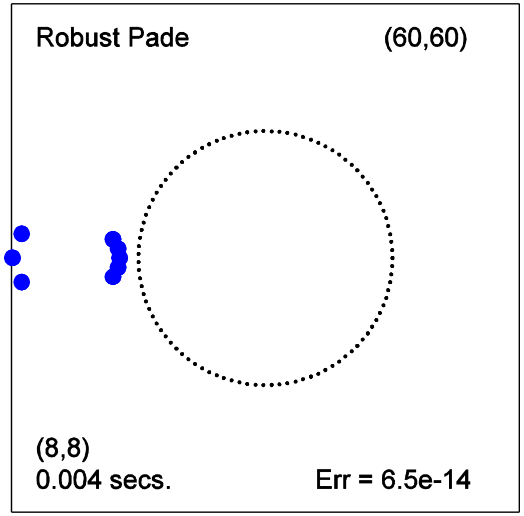
log(1.2−z), type (20,20)





$\mathrm{Exp}((z+1.5)^{-2})$, type (60,60)





SPURIOUS POLES/FROISSART DOUBLETS

The pink & red dots are poles with very small residue, typically due to rounding. Equivalently: pole/zero pairs with very small separation, called Froissart doublets.

Theoretical (exact arithmetic) literature: because of doublets, one gets only convergence in capacity in (n,n) Padé approx as $n \to \infty$ (Nuttall 1970, Pommerenke 1973, Stahl 1997, Suetin 2010).

cf. talk by Aptekarev going on right now in Alvania room

Computation: numerical doublets are ubiquitous, caused by singular vals $\sigma \approx 0$.

We think the new algorithm may be interesting for theory as well as computation.

A THEORETICAL CHALLENGE

The literature seems to accept that rational approx is intrinsically delicate, so any theory must be delicate too, and computations are "art, not science".

Stahl, 2006: *"Spurious poles... are a phenomenon that unfortunately cannot be ignored in Padé approximation."*

Yet our alg. with TOL = 10^{-14} eliminates poles introduced by rounding errors.

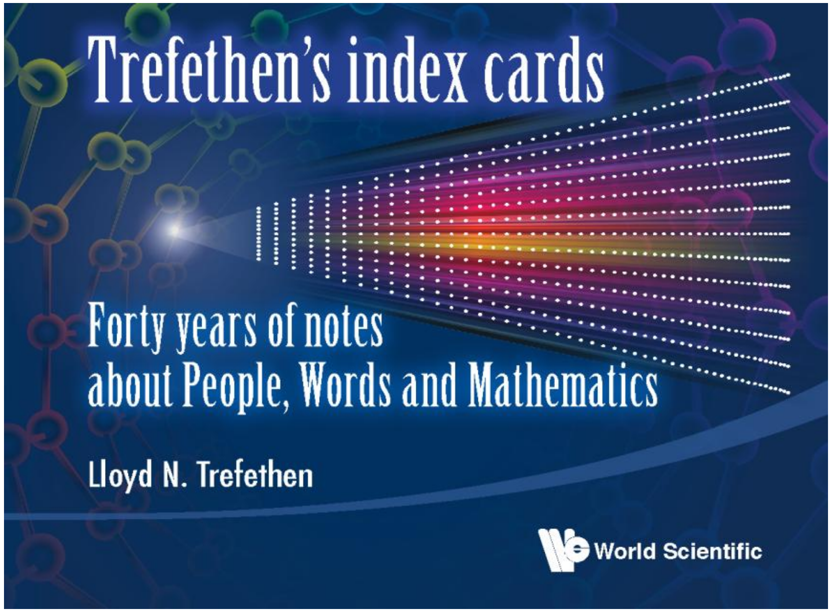
What about an approximation defined by SVD with TOL $\rightarrow 0$ as $n \rightarrow \infty$?

Can one define a robust Padé approximant with true pointwise convergence?

Finally, two advertisements

1: Chebfun demo tomorrow 12:30 (Alvania room)

2: Check out my new book on display at Springer desk!
(available from publisher or from amazon)



THANK YOU!