Matrix functions, quadrature formulas, and rational approximation

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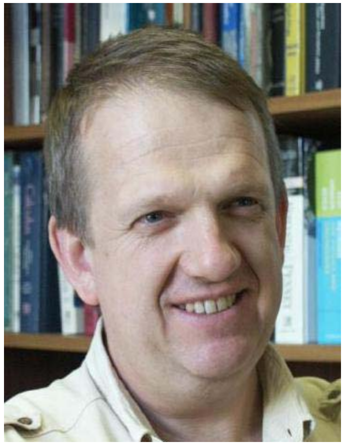
With thanks to



André Weideman
U. Stellenbosch

Thomas Schmelzer
Oxford DPhil 2007

W., "Optimizing Talbot's Contours for the Inversion of the Laplace Transform", *SINUM,* 2006

T. + W. + S., "Talbot quadratures and rational approximations", *BIT,* 2006 ←

W. + T., "Parabolic and hyperbolic contours for computing the Bromwich integral", *Math. Comp.*, 2007

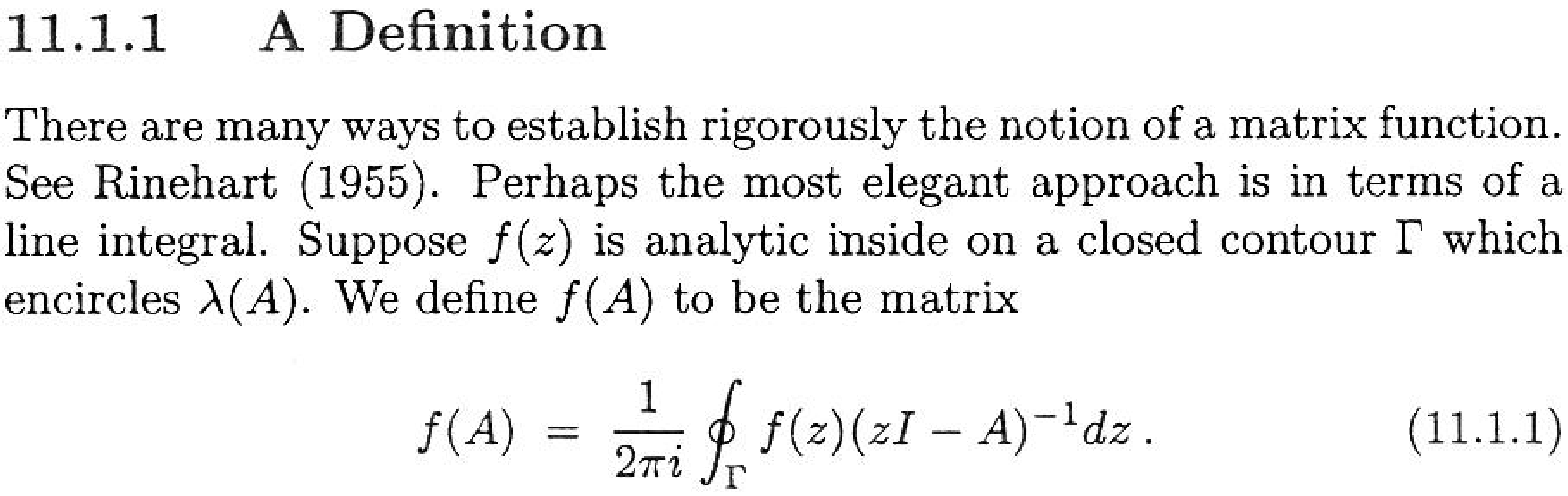
S. + T., "Computing the gamma function using contour integrals and ratl. approxs.", *SINUM,* 2007

S. + T., "Evaluating matrix functions for exponential integrators...", *ETNA*, 2007

W., "Improved contour integral methods for parabolic PDEs", *IMAJNA,* to appear

1. Cauchy integral + trapezoid rule = $f(A)$

From Golub & Van Loan:

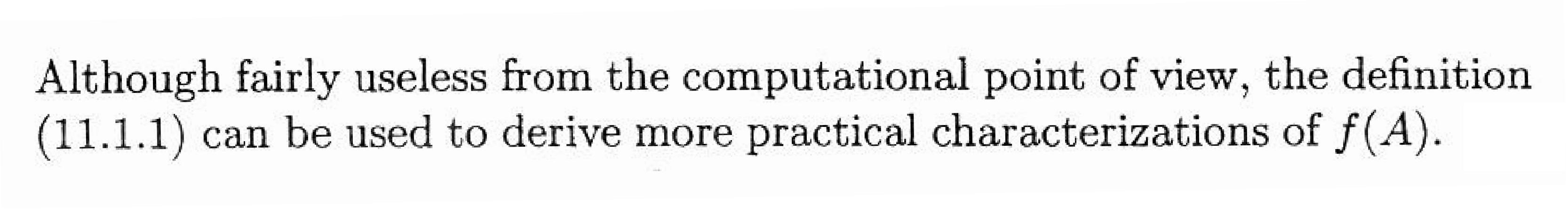


11.1.1 A Definition

There are many ways to establish rigorously the notion of a matrix function. See Rinehart (1955). Perhaps the most elegant approach is in terms of a line integral. Suppose $f(z)$ is analytic inside on a closed contour Γ which encircles $\lambda(A)$. We define $f(A)$ to be the matrix

$$f(A) = \frac{1}{2\pi i}\oint_{\Gamma} f(z)(zI - A)^{-1} dz\,. \tag{11.1.1}$$

They go on to say...

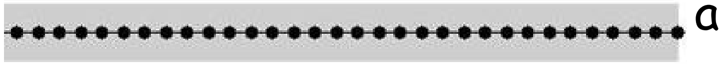


Although fairly useless from the computational point of view, the definition (11.1.1) can be used to derive more practical characterizations of $f(A)$.

Exponential accuracy of trapezoid rule for analytic functions

Periodic interval

Poisson 1826, Davis 1959



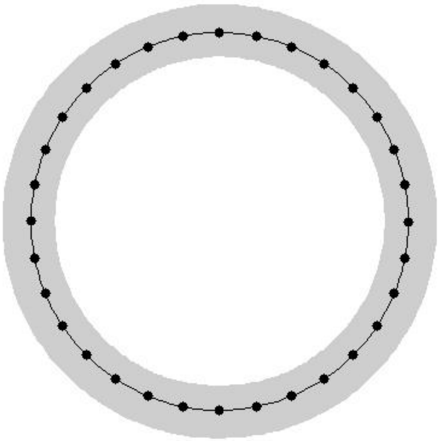
Real line

Turing 1943, Goodwin 1949,
Martensen 1968, Stenger 1981

error $e^{-2\pi a/\Delta x}$

Circle

Davis 1959



If the Cauchy integral
contour Γ is circular,
the trapezoid rule
should be superb !

Toy example—computing $J_0(A)$ for a 3x3 random A

```
f = @(z)  besselj(0,z);
A = randn(3)/4;  I = eye(3);
for n = 10:10:40
      z = exp(2i*pi*(1:n)/n);
      B = zeros(3);
      for i = 1:n,  B = B + inv(z(i)*I-A)*z(i)*f(z(i))/n;  end
      n, B
end
```

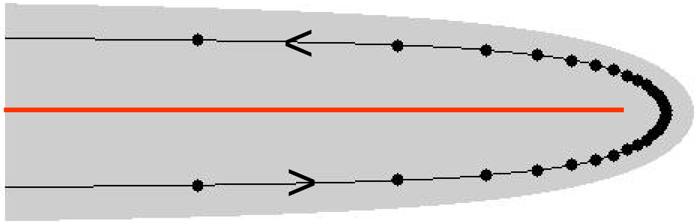
fA.m

2. Talbot contours for f = exp and other integrals involving exp(z)

A special case of a Cauchy integral is the inverse Laplace transform e^A of $(z-A)^{-1}$:

"Bromwich integral"

$$\boxed{e^A = \frac{1}{2\pi i}\int_C (z-A)^{-1} e^z \, dz}$$



C winds around $(-\infty, 0]$

To a Laplace transform person, this is a relationship $e^A \leftrightarrow (z-A)^{-1}$.

To a resolvent integrals person, it is a relationship $e^A \leftrightarrow e^z$.

This formula is valid if A is a matrix or hermitian operator with spectrum ≤ 0. Generalizations e.g. to sectorial operators.

For this and similar problems with e^z in the integrand, we shall explore two types of method:

TW = Talbot/Weideman	based on quadrature formulas on contour
CMV = Cody-Meinardus-Varga	based on best approximation of e^z on $(-\infty, 0]$

TALBOT-WEIDEMAN COTANGENT CONTOUR

Talbot (1979) proposed transplanting the trap. rule from [−π,π]:

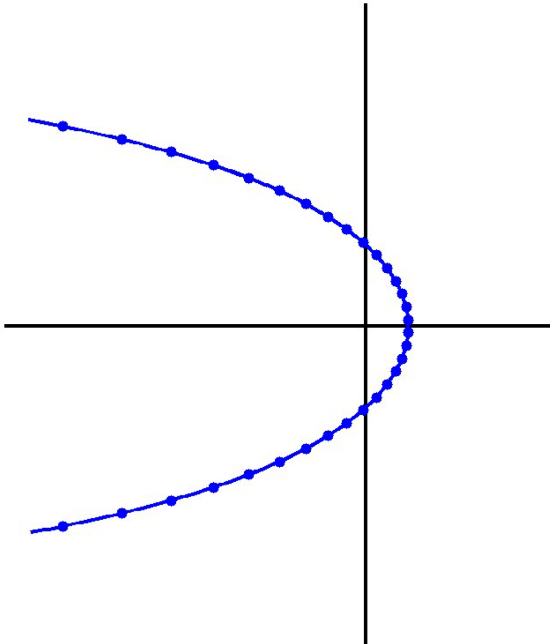
$$z(\theta) \;=\; \sigma + \mu(\theta\cot\theta + \nu i\theta)$$

Weideman (2005) optimized the parameters:

$$z(\theta) \;=\; N\,[\,0.5017\,\theta\cot(0.6407\,\theta) - 0.6122 + 0.2645\,i\,\theta\,]$$

with the exponential convergence rate

$$\text{Error} \;\approx\; e^{-1.36N} \approx \boxed{3.89^{-N}}$$



Weideman has also found an optimal PARABOLIC CONTOUR

$$z(\theta) \;=\; N\left[0.1309 - 0.1194\theta^2 + 0.2500\,i\,\theta\right]$$

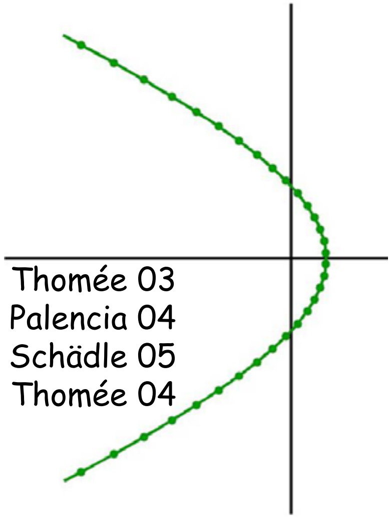
with convergence rate

$$\text{Error} \;\approx\; e^{-1.05N} \approx \boxed{2.85^{-N}}$$

cf. Sheen & Sloan & Thomée 99
Gavrilyuk & Makarov 01

and an optimal HYPERBOLIC CONTOUR

$$z(\theta) \;=\; 2.246N\left[1 - \sin(1.1721 - 0.3443i\theta)\right]$$



with convergence rate

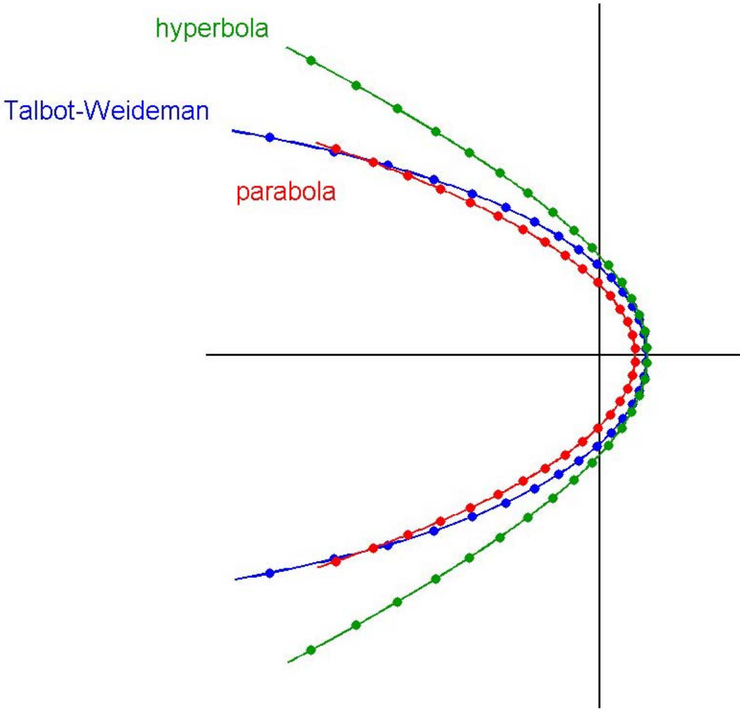
$$\text{Error} \;\approx\; e^{-1.16N} \approx \boxed{3.20^{-N}}$$

cf. Sheen & Sloan & Thomée 03
López-Fernández & Palencia 04
López-Fernández & Palencia & Schädle 05
McLean & Thomée 04

These formulas are again written for $\theta \in [-\pi,\pi]$.
(Artificial periodicity: exponentially small integrand at $|\theta| \approx \pi$.)

3. Quadrature = rational approximation

INTERPRETATION AS RATIONAL APPROXIMATIONS TO e^z



Suppose we approximate by quadrature

$$\frac{1}{2\pi i}\int_C e^z f(z)\,dz \approx \sum_{k=1}^{N} c_k\, e^{z_k} f(z_k)$$

where $f(z)$ is analytic for $z \notin (-\infty, 0]$.
By residue calculus we can interpret this sum as

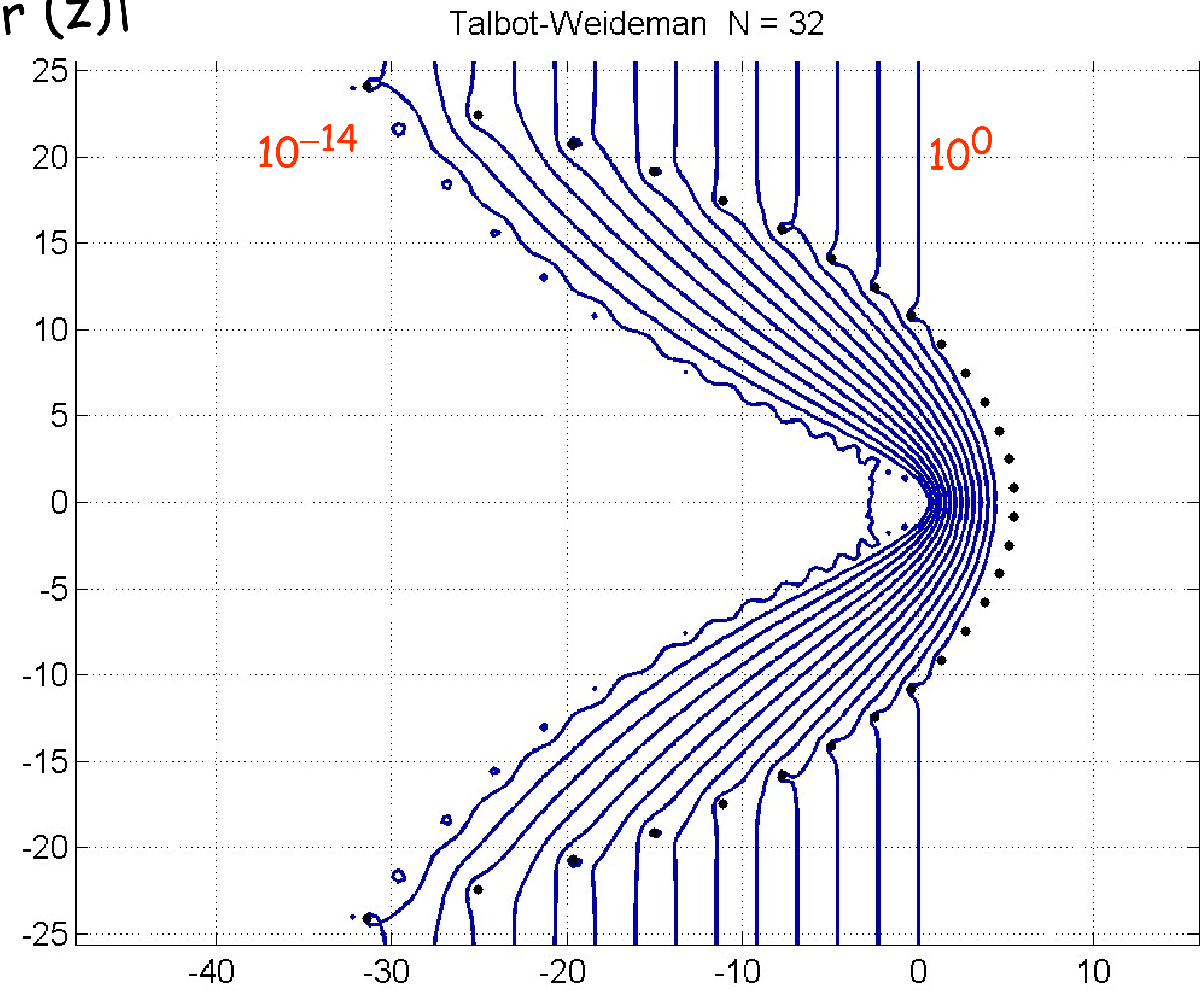
$$\frac{1}{2\pi i}\int_C r(z) f(z)\,dz\,, \qquad r(z) = -\sum_{k=1}^{N}\frac{c_k e^{z_k}}{z - z_k}$$

assuming $|f(z)| \to 0$ as $|z| \to \infty$. In particular if $z = z(\theta)$ and we use the trapezoid rule for $\theta \in [-\pi, \pi]$, we get

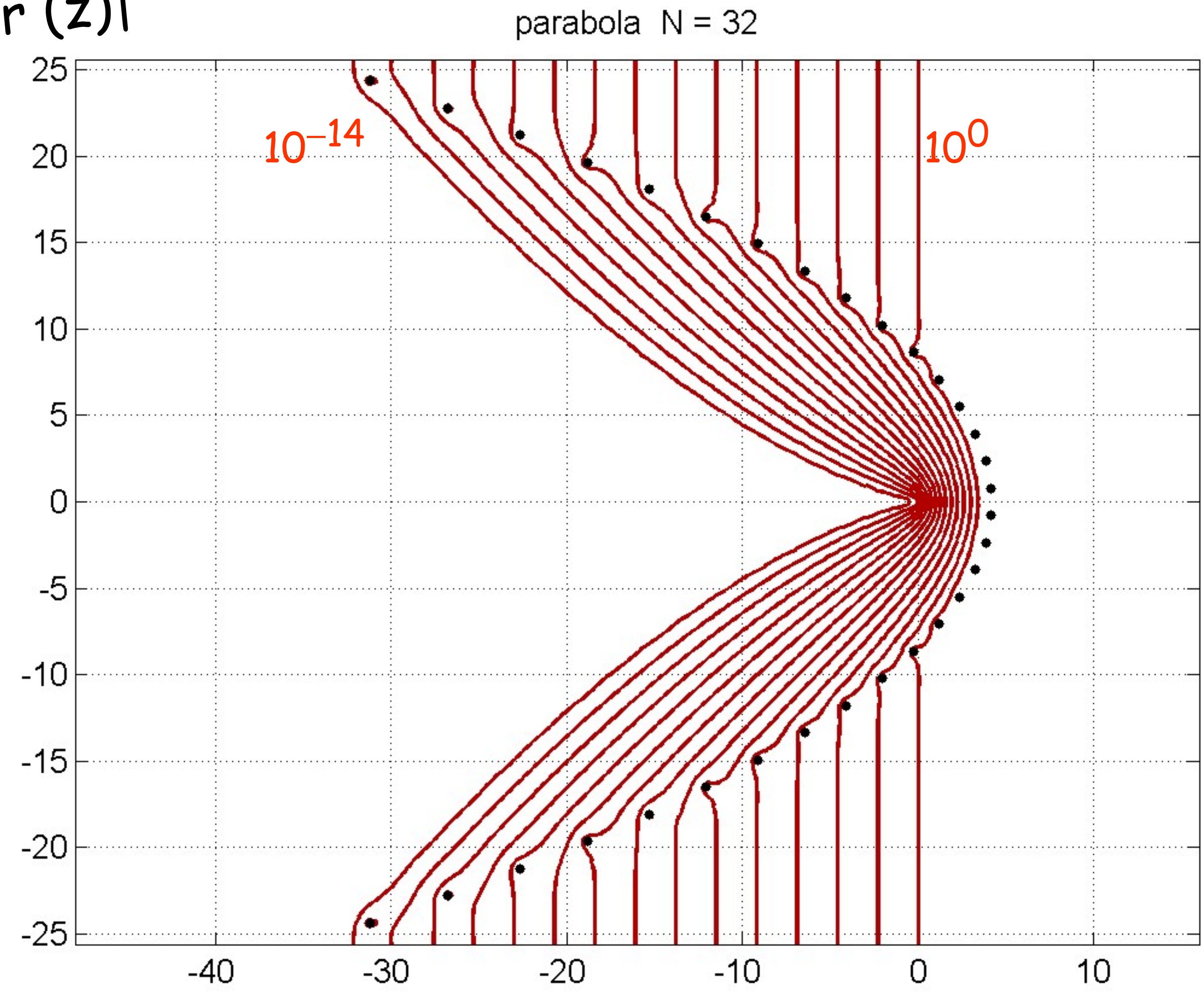
$$c_k = \frac{-i}{N}(dz/d\theta)_k\,, \qquad \boxed{r(z) = \frac{i}{N}\sum_{k=1}^{N}\frac{e^{z_k}(dz/d\theta)_k}{z - z_k}}$$

type $(N-1,\ N)$ rational approximation to e^z

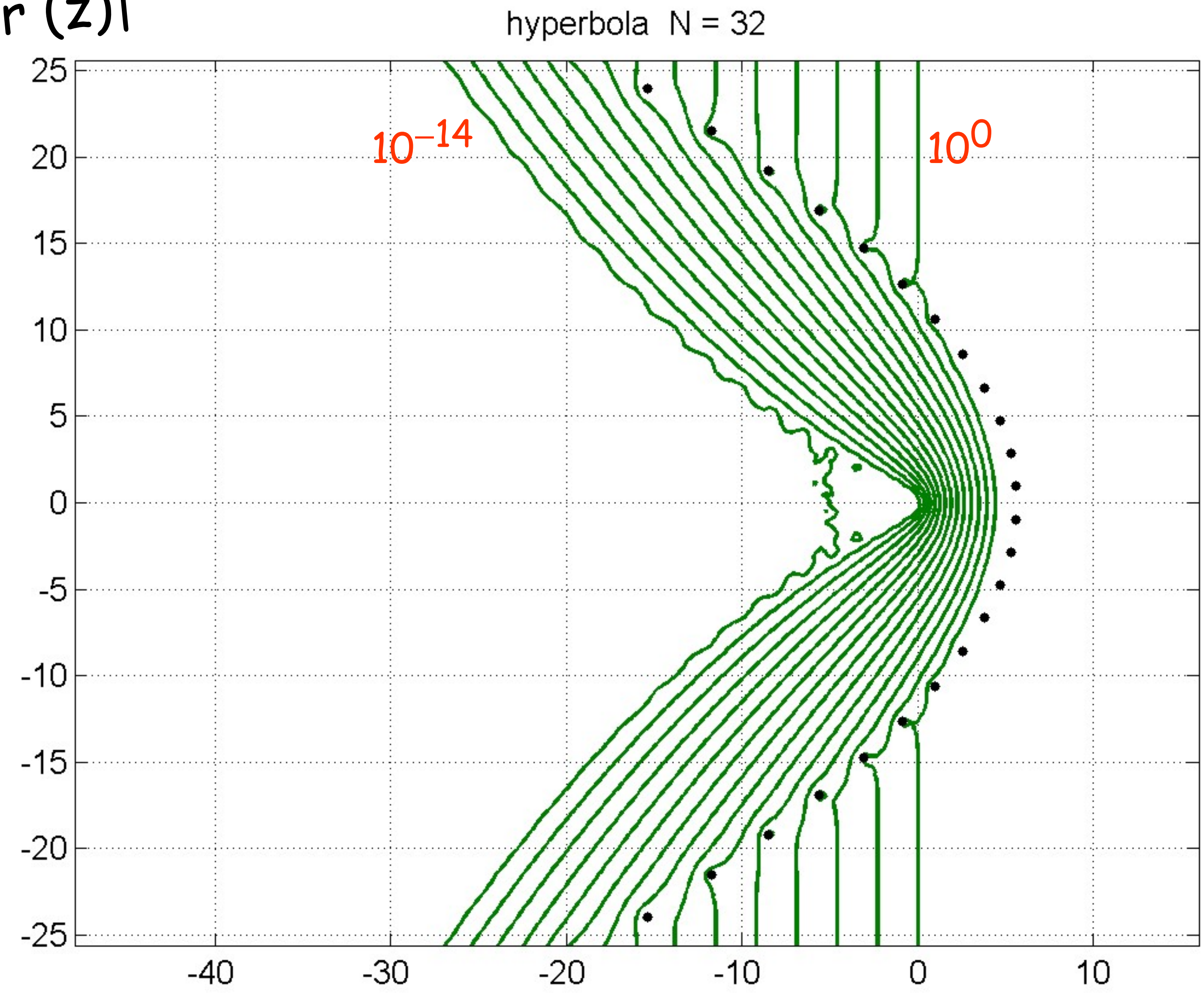
$|e^z - r(z)|$


Talbot-Weideman N = 32
10^{-14}
10^{0}
25
20
15
10
5
0
-5
-10
-15
-20
-25
-40
-30
-20
-10
0
10

$|e^z - r(z)|$



$|e^z - r(z)|$



USE OF BEST APPROXIMATIONS ON $(-\infty,0]$

Instead of obtaining rational approximants implicitly from quadrature formulas, we could construct them directly.

Cody, Meinardus & Varga (1969) made famous the problem of best approximation of e^z in the sup-norm on $(-\infty,0]$.

Here the convergence rate is famous:

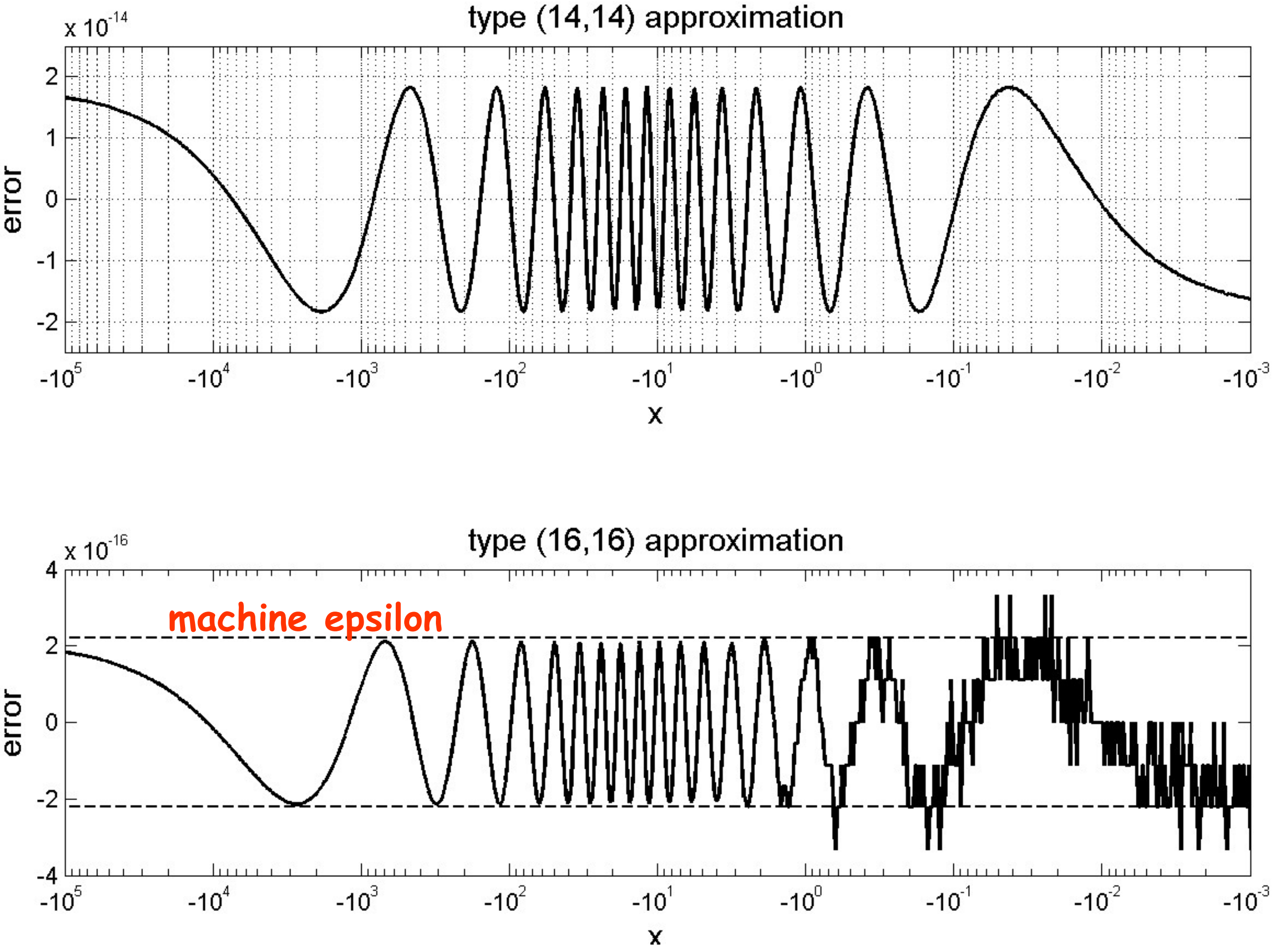
$$\text{Error} \approx e^{-2.2288N} \approx \boxed{9.28903^{-N}}$$

Gonchar & Rakhmanov 1987

Aptekarev, Magnus, Saff, Stahl, Totik, …

Notice this is around twice as fast as for the quadrature methods.

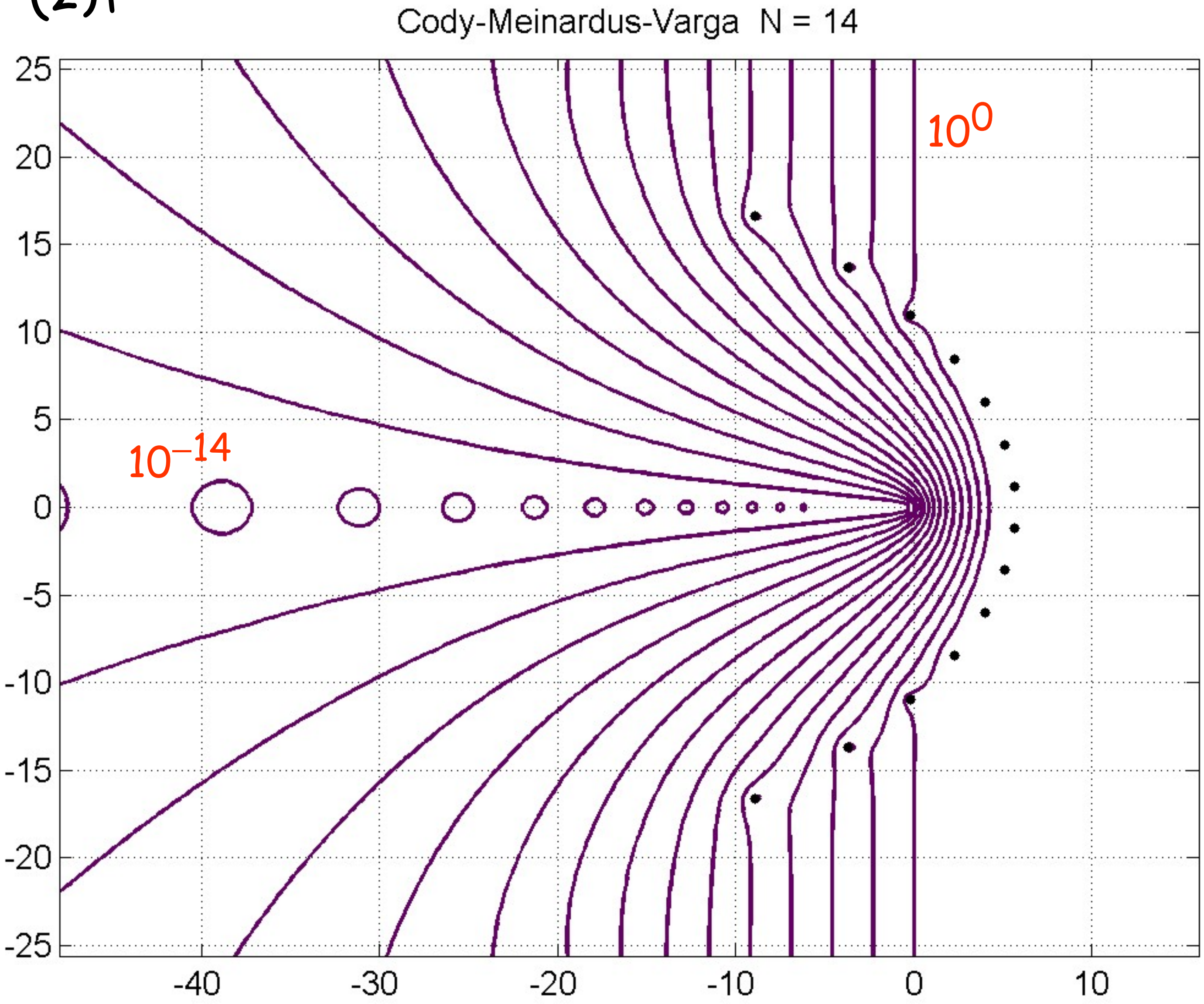
Some CMV best approximation error curves

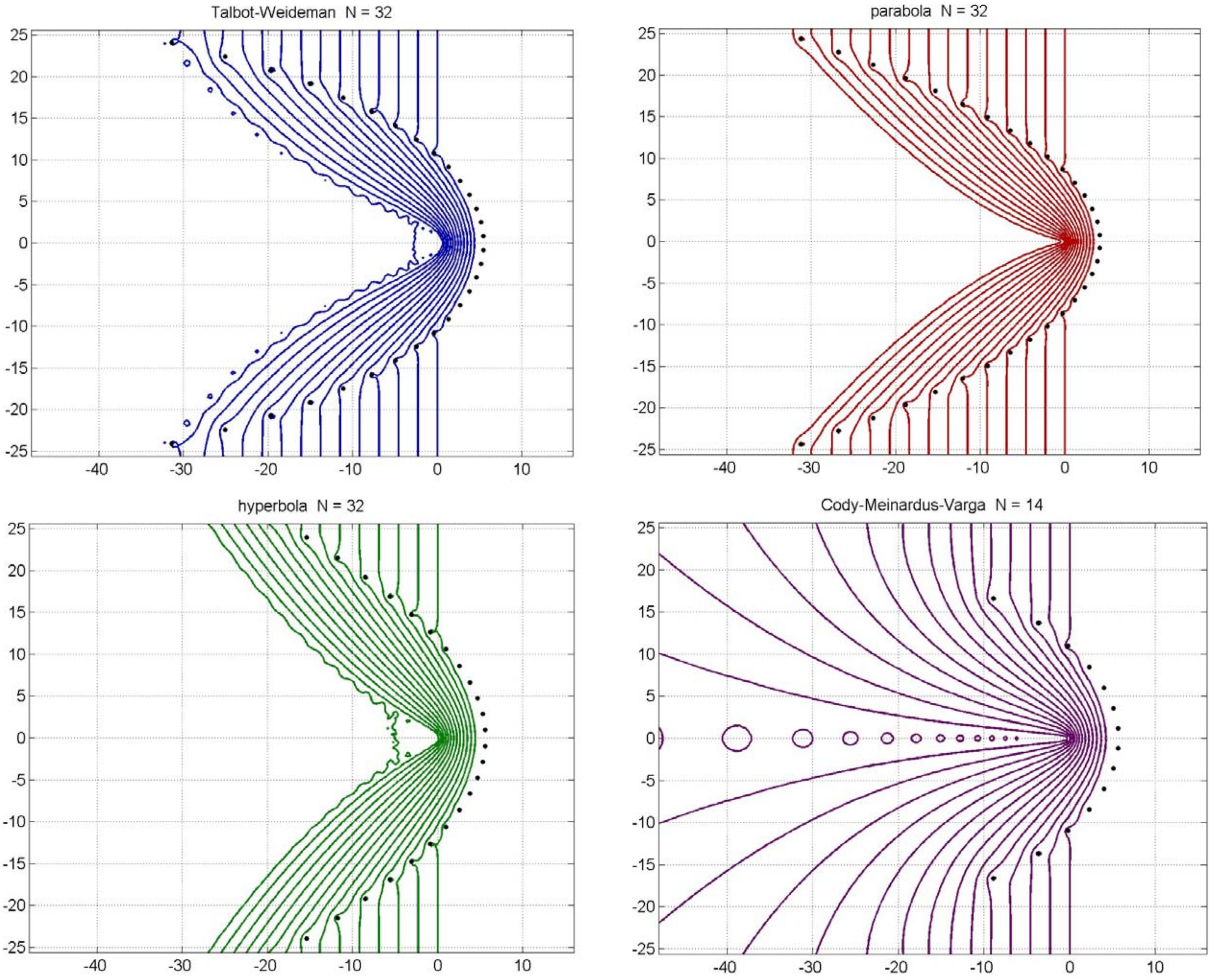


In practice we can compute these approximants easily with CF = Carathéodory-Fejér approximation, based on SVD of Hankel matrix of transplanted Chebyshev coefficients.

expx_cf.m

$|e^z - r(z)|$


Cody-Meinardus-Varga N = 14
10^0
10^{-14}
25
20
15
10
5
0
-5
-10
-15
-20
-25
-40
-30
-20
-10
0
10


Talbot-Weideman N = 32
parabola N = 32
hyperbola N = 32
Cody-Meinardus-Varga N = 14
25
20
15
10
5
0
-5
-10
-15
-20
-25
-40
-30
-20
-10
0
10

SUMMARY OF THE TWO APPROACHES

Given: inverse Laplace integral $g = \int_C f(z)\, e^z \, dz$

(C winds around $(-\infty, 0]$)

Best approximation ("CMV")

(1) Replace e^z by $r(z)$

(2) Deform C to contour Γ enclosing poles

(3) Evaluate integral by residue calculus

Quadrature contours ("TW")

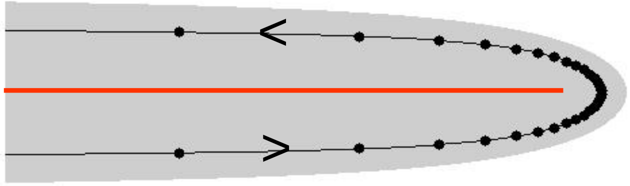
(1) Deform C to contour Γ

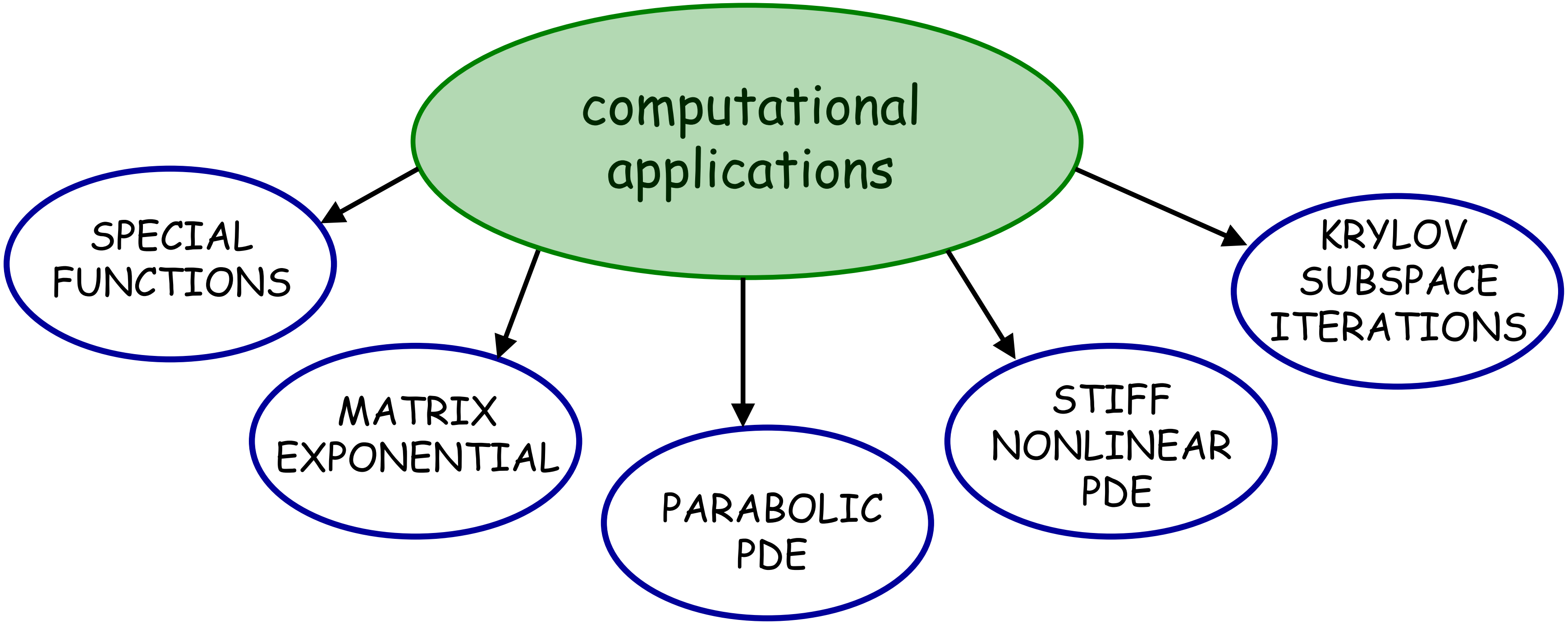
(2) Evaluate integral by quadrature formula (typically trapezoid rule after change of variables)

(3) Interpret this as evaluation by residues of a contour integral involving a rational function $r(z)$

$$\boxed{e^A = \frac{1}{2\pi i}\int_C (z - A)^{-1} e^z \, dz}$$

and similar integrals





computational applications

SPECIAL FUNCTIONS

MATRIX EXPONENTIAL

PARABOLIC PDE

STIFF NONLINEAR PDE

KRYLOV SUBSPACE ITERATIONS

	TW = quadrature over contours	CMV = best approximation on $(-\infty, 0]$
Laplace transforms & special functions	Luke 69 Talbot 79 Temme 96 Gil & Segura & Temme 02	Schmelzer & T. 07
matrix exponential (e^A or $e^A v$)	Sidje 98 Kellems 05	Lu 98
parabolic PDE	Gavrilyuk & Makarov 01 Sheen & Sloan & Thomée 99 & 03 Mclean & Thomée 04 López-Fernández & Palencia 04	Varga 61 Cody & Meinardus & Varga 69 Cavendish & Culham & Varga 84 Gallopoulos & Saad 89, 92
stiff nonlinear PDE	Kassam & T. 03	Lu 05
Krylov subspace its.		Gallopoulos & Saad 89, 92

+ much related work by Baldwin, Calvetti, Druskin, Eiermann, Freund, Hochbruck, Knizhnerman, Krogstad, Lubich, Minchev, Moret, Novarti, Ostermann, Reichel, Sadkane, Schädle, Sorensen, Tuckerman, Tal-Ezer, Wright…

IN CONCLUSION

Rational approximations, quadrature formulas, the complex plane... these sound old-fashioned!

Still, they are the basis of powerful algorithms for f(A) and f(A)b.

Two big advantages: f(A)b is easy; minimal dependence on f

We've considered entire functions f.

For more complicated functions, see next talk by Nick Hale.