Talbot quadratures and rational approximations

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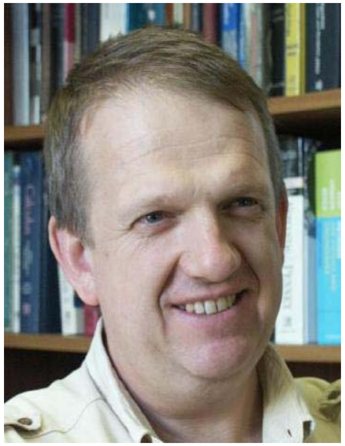
With thanks to



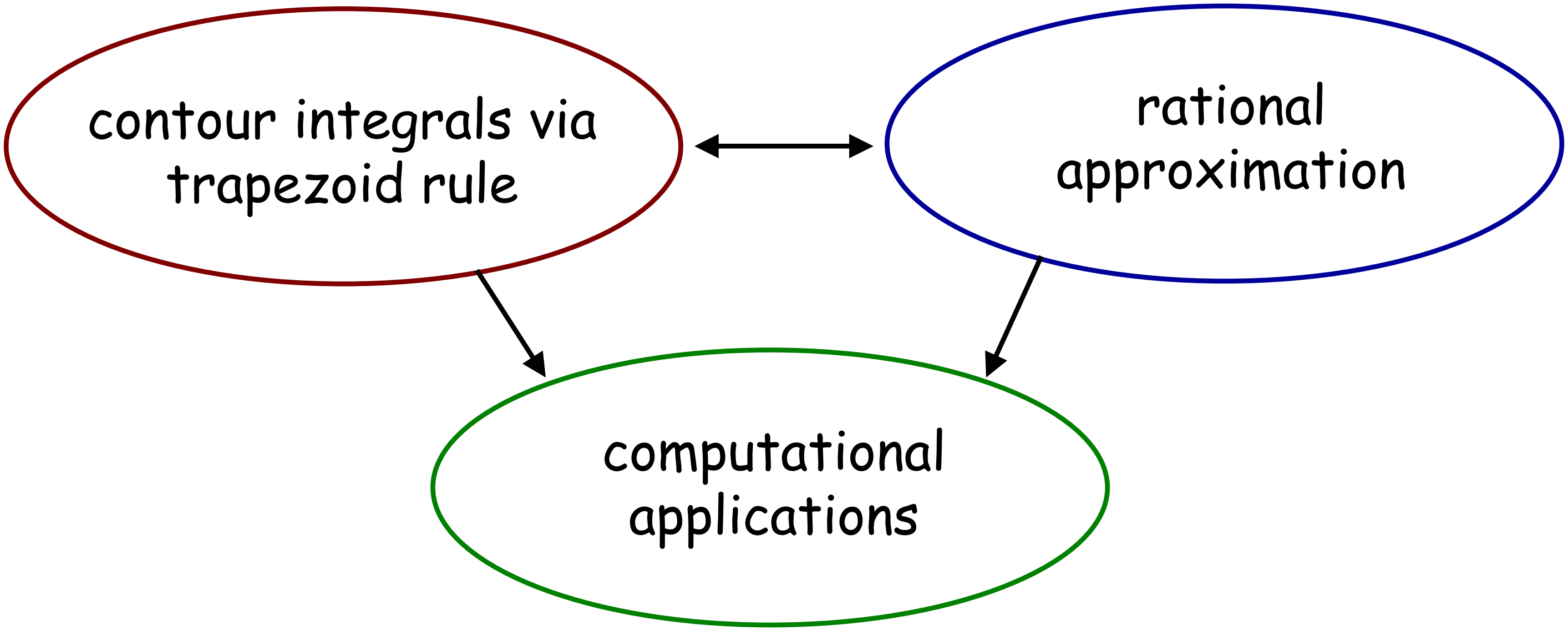
talk today at 14.45 !

André Weideman
Stellenbosch

Thomas Schmelzer
Oxford

T. + Weideman + Schmelzer, "Talbot quadratures and rational approximations", *BIT*, to appear

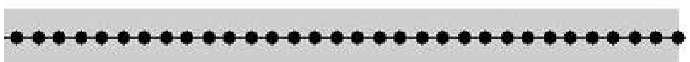
Weideman + T., "Parabolic and hyperbolic contours for computing the Bromwich integral", *Math. Comp.*, to appear


contour integrals via trapezoid rule
rational approximation
computational applications

contour integrals via trapezoid rule

Exponential accuracy of trapezoid rule for analytic functions

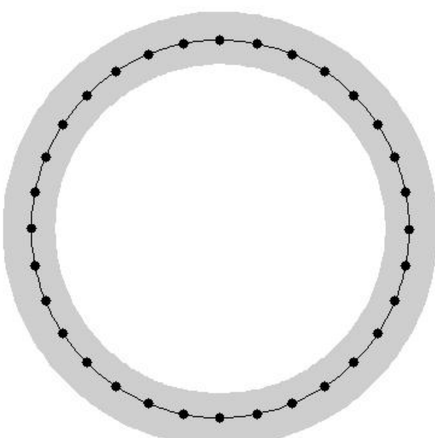
Periodic interval
Poisson 1826, Davis 1959



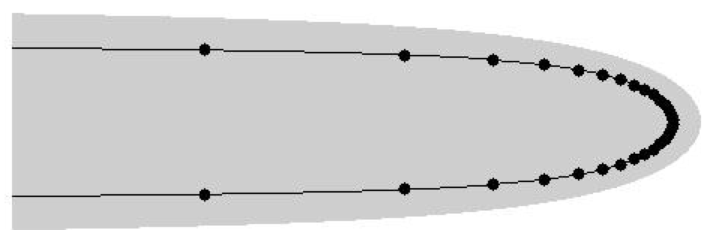
Real line
Turing 1943, Goodwin 1949, Martensen 1968, Stenger 1981

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

Circle
Davis 1959



Inverse Laplace transform contour
Talbot 1979, Weideman 2005



(trap. rule after change of variables)

In complex analysis a particular interest is Cauchy integrals

rational approximation

$$f(a) = \frac{1}{2\pi i}\int_C \frac{f(z)}{z-a}\,dz$$

where C encloses a, or for a matrix or operator,

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

resolvent integral

where C encloses spec(A). Use of a quadrature formula such as the trapezoid rule turns these into rational approximations:

r(a)

$$f(a) \approx \boxed{\frac{1}{2\pi i}\sum_k \frac{c_k f(z_k)}{z_k - a}}$$

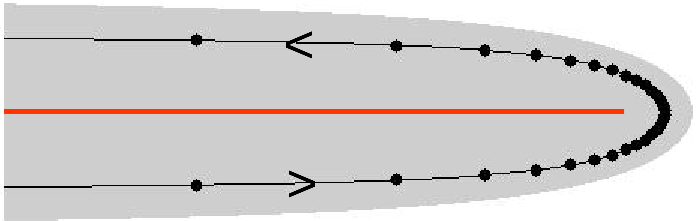
r(A)

$$f(A) \approx \boxed{\frac{1}{2\pi i}\sum_k c_k f(z_k)(z_k - A)^{-1}}$$

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

"Bromwich integral"

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



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

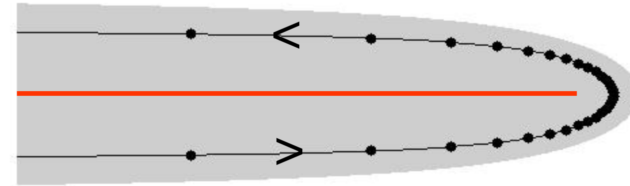
This formula is valid if A is a matrix or hermitian operator with spectrum ≤ 0. Generalizations e.g. to sectorial operators.

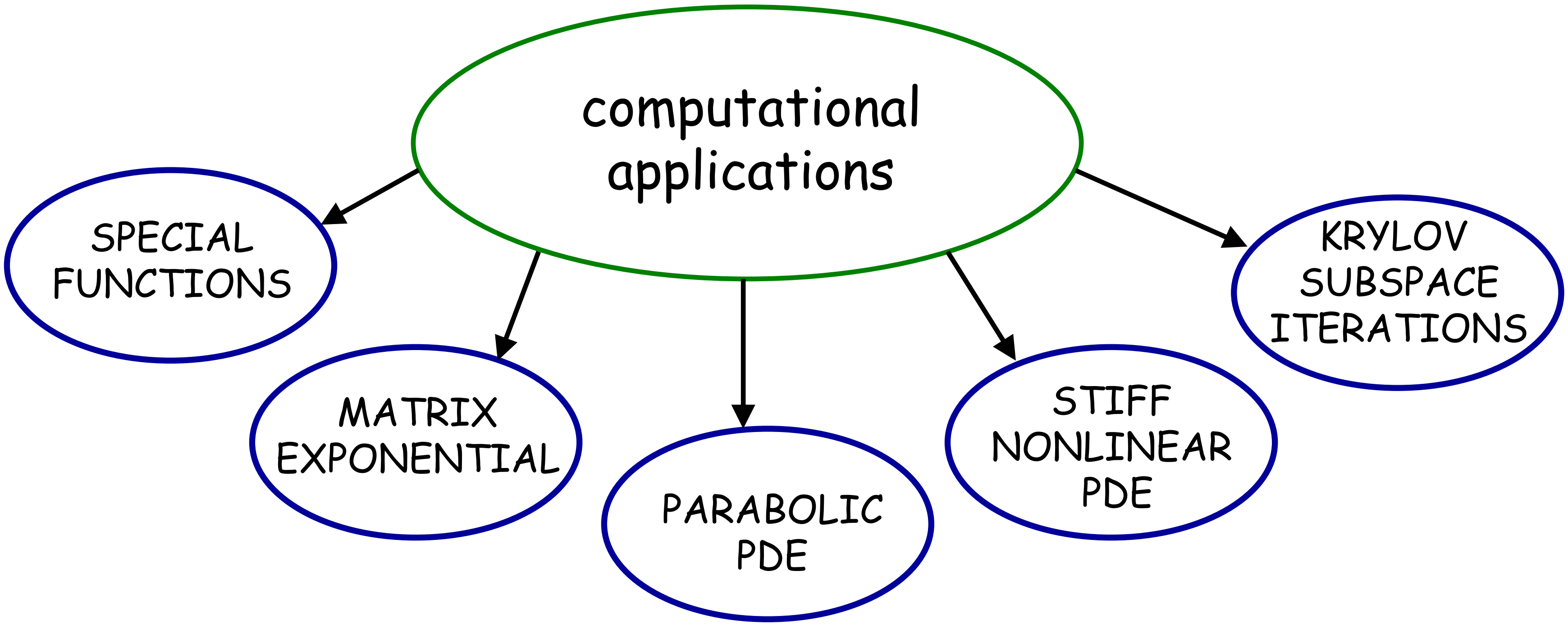
This talk is about this and similar problems with e^z or e^{tz} in the integrand, for which we consider two types of numerical method:

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

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

and similar integrals





Plan for the rest of the talk:
(1) Describe and compare TW contours vs. CMV best approxs.
(2) Show a couple of computed examples

TALBOT-WEIDEMAN COTANGENT CONTOUR

Talbot (1979) proposed transplanting the trap. rule from [$-\pi,\pi$]:

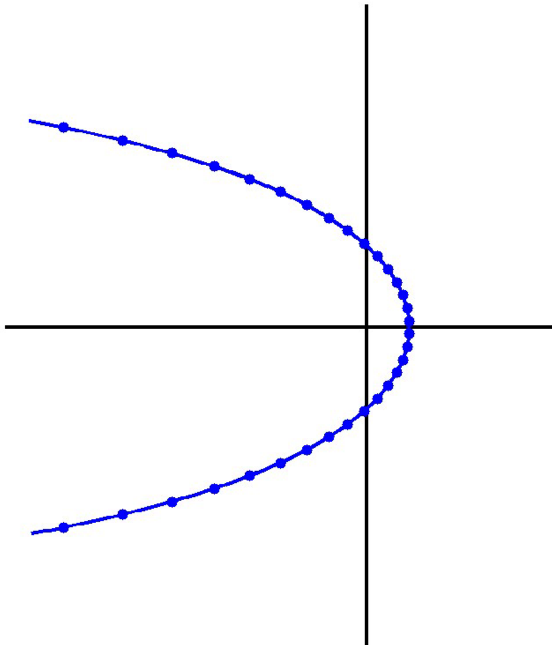
$$z(\theta) \;=\; \sigma + \mu(\theta\cot\theta + \nu i\theta)$$

Weideman (2005) optimized the parameters:

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

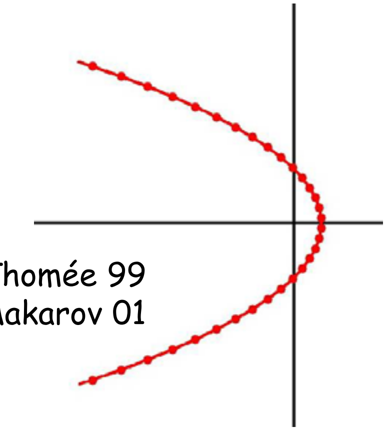
with the exponential convergence rate

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



Weideman has also found an optimal PARABOLIC CONTOUR

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



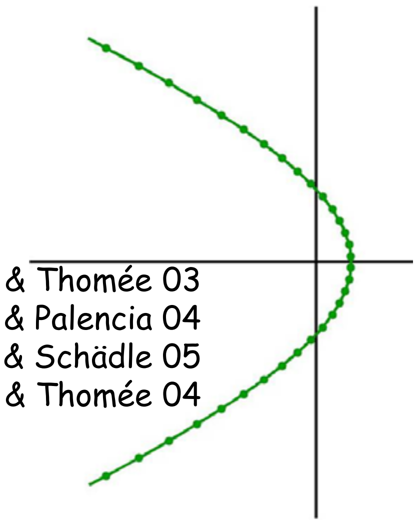
with convergence rate

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

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

and an optimal HYPERBOLIC CONTOUR

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



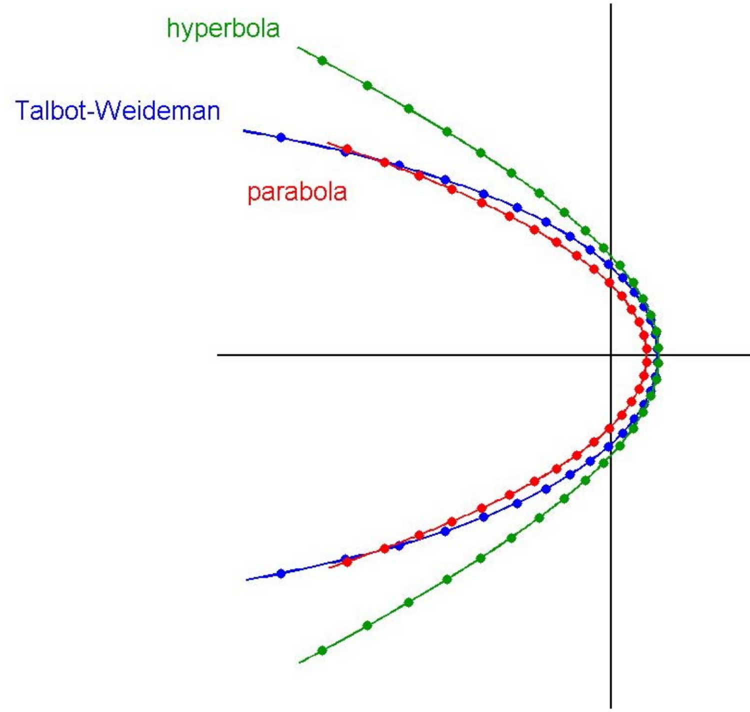
with convergence rate

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

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 $|\theta| \approx \pi$.)

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

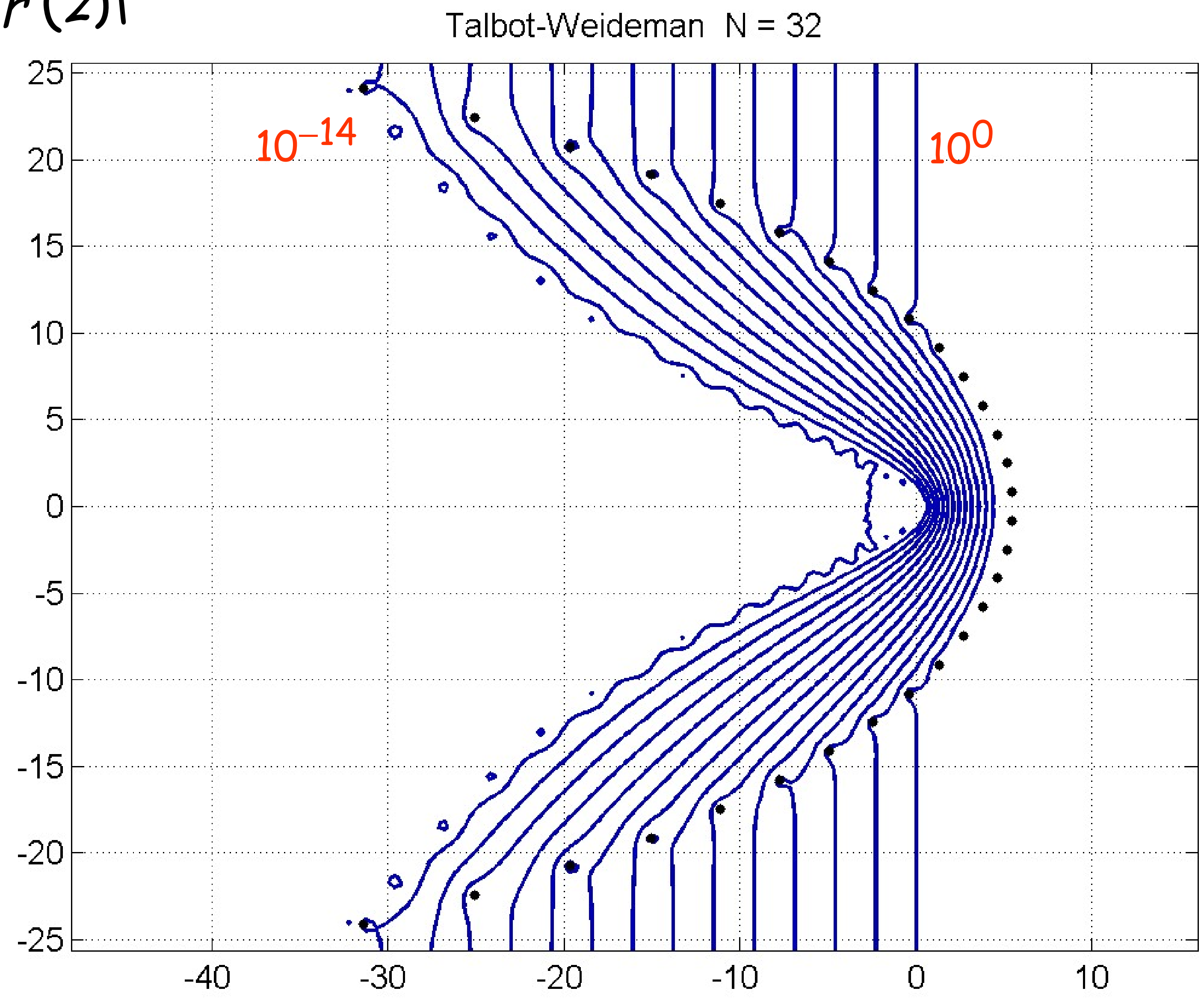
$$\frac{1}{2\pi i}\int_C r(z) f(z)\,dz\,, \qquad r(z) = -\sum_{k=1}^{N} \frac{c_k e^{z_k}}{z - z_k}$$

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

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

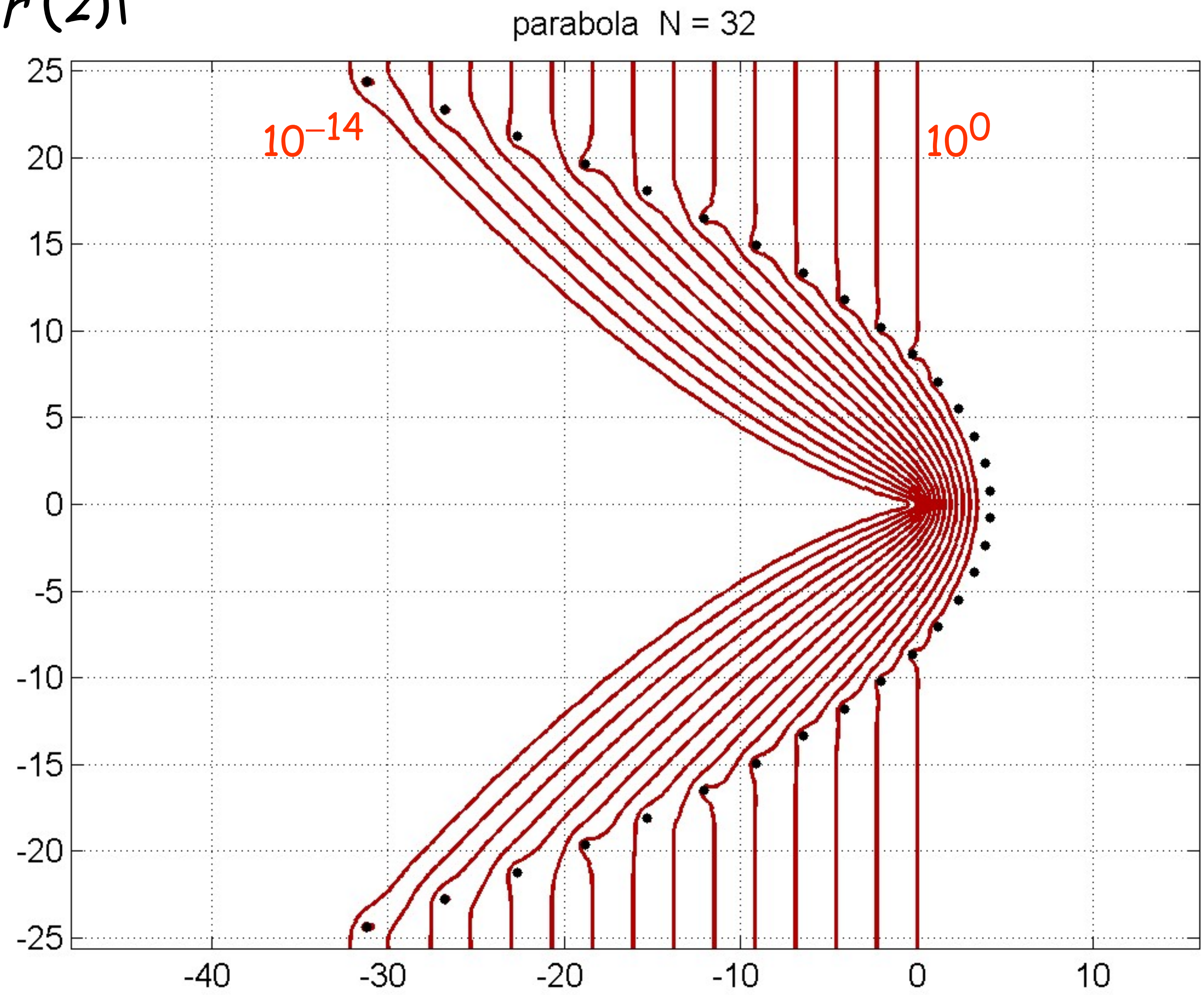
type $(N-1, N)$ rational approximation to e^z

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

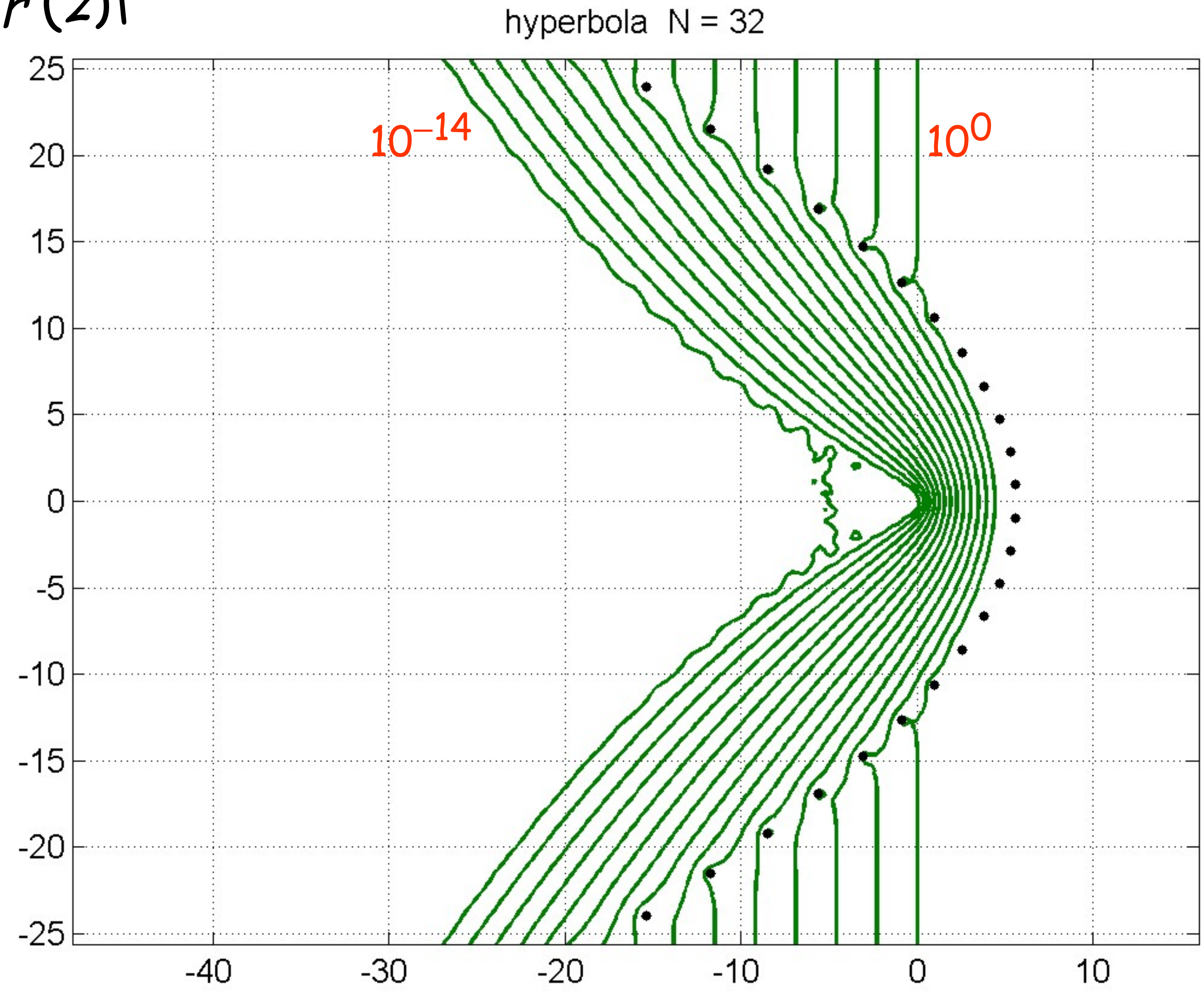


Talbot-Weideman N = 32
10^-14
10^0
25
20
15
10
5
0
-5
-10
-15
-20
-25
-40
-30
-20
-10
0
10

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



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



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:

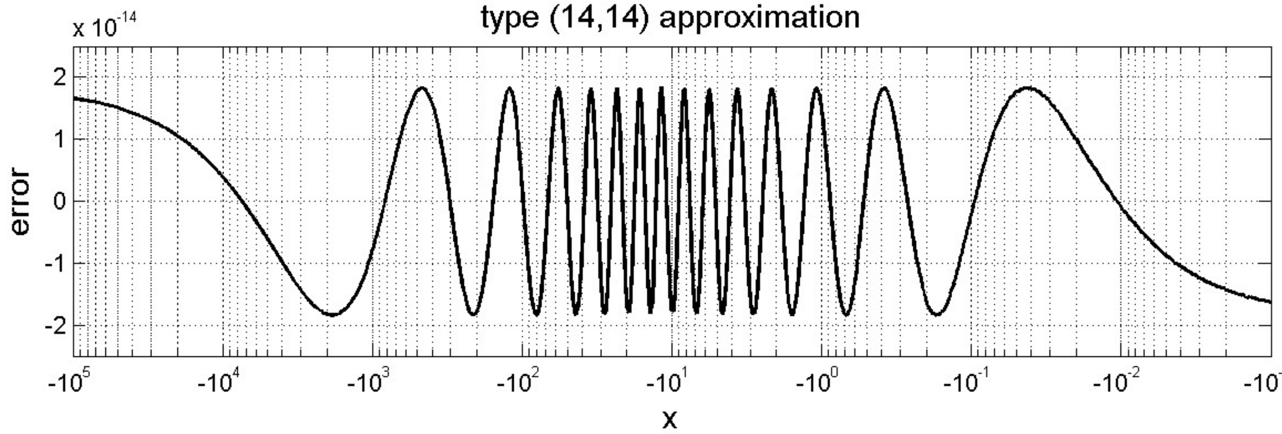
Gonchar & Rakhmanov 1987

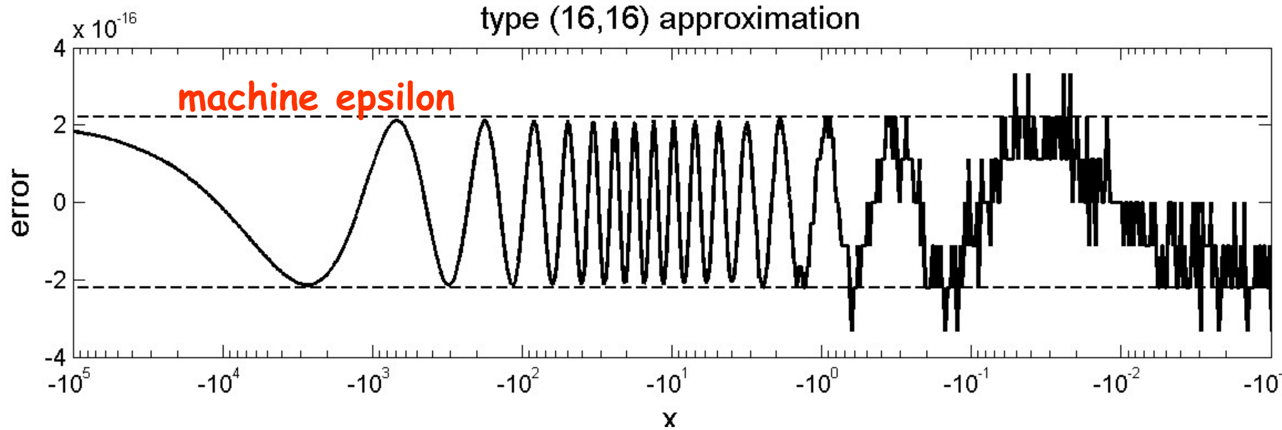
$$\text{Error} \approx e^{-2.2288N} \approx 9.28903^{-N}$$

Aptekarev, Magnus, Saff, Stahl, Totik, …

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

Some CMV best approximation error curves

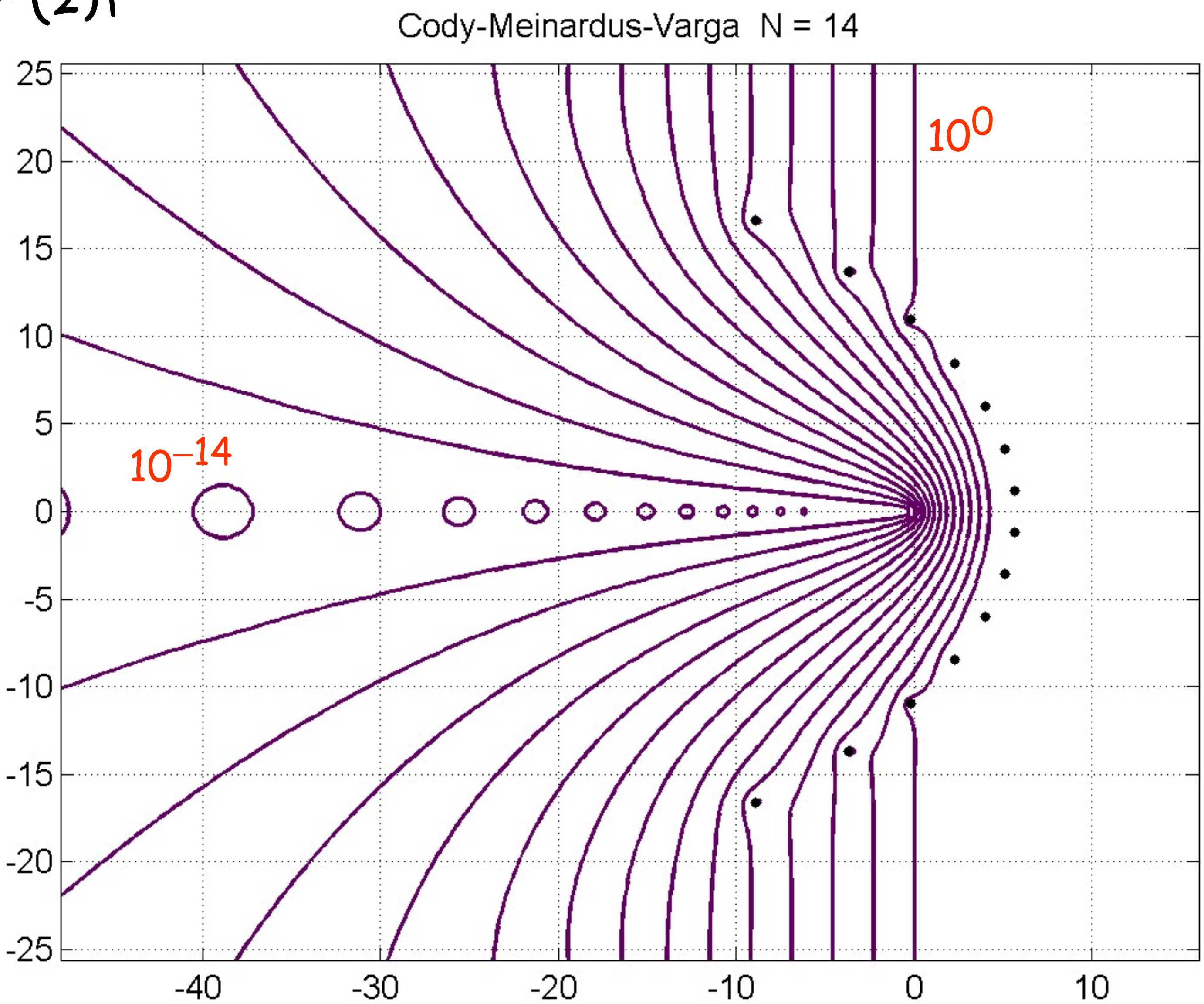




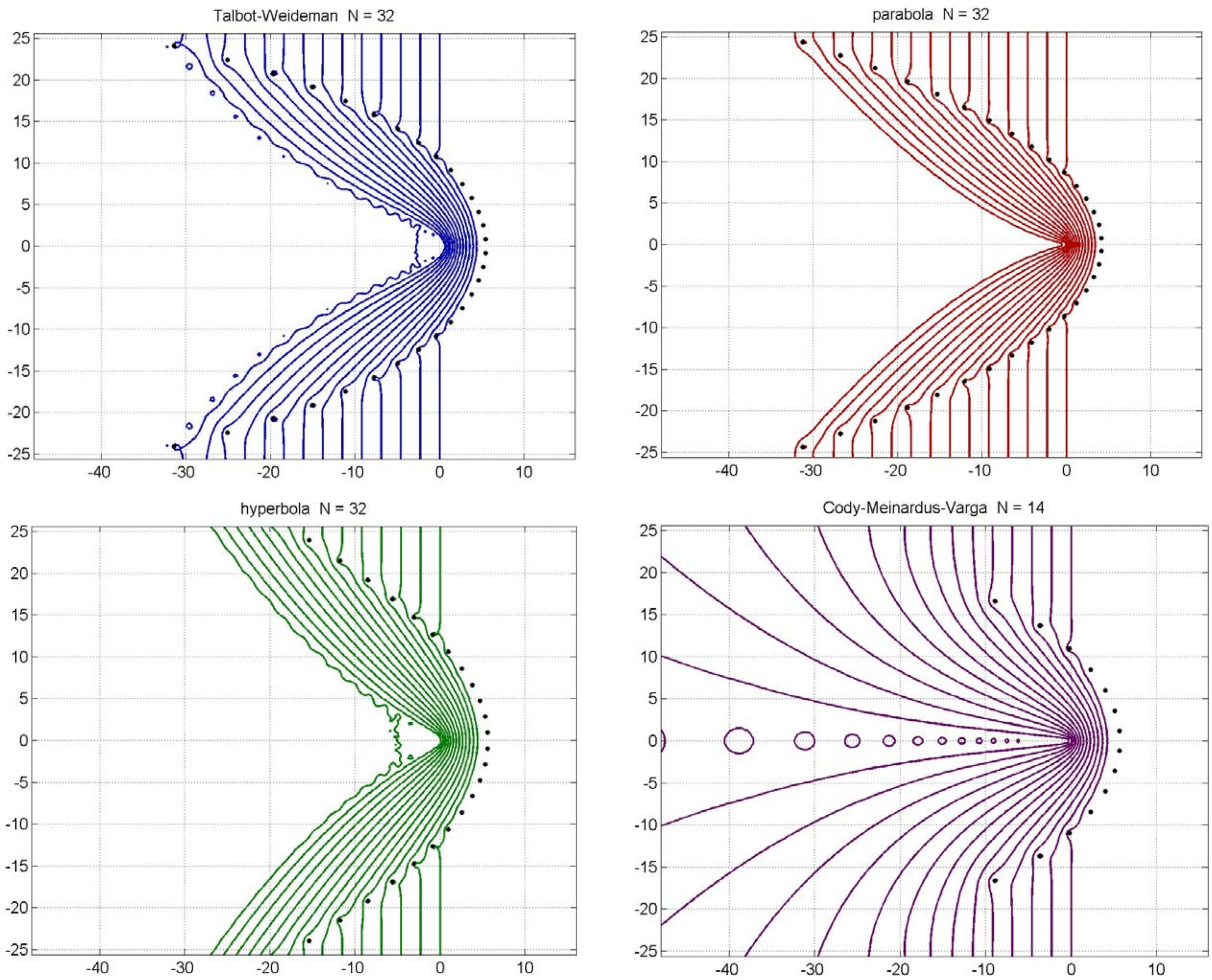
In practice we can compute these approximants effortlessly with CF = Carathéodory-Fejér approximation, based on SVD of Hankel matrix of transplanted Chebyshev coefficients.

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")

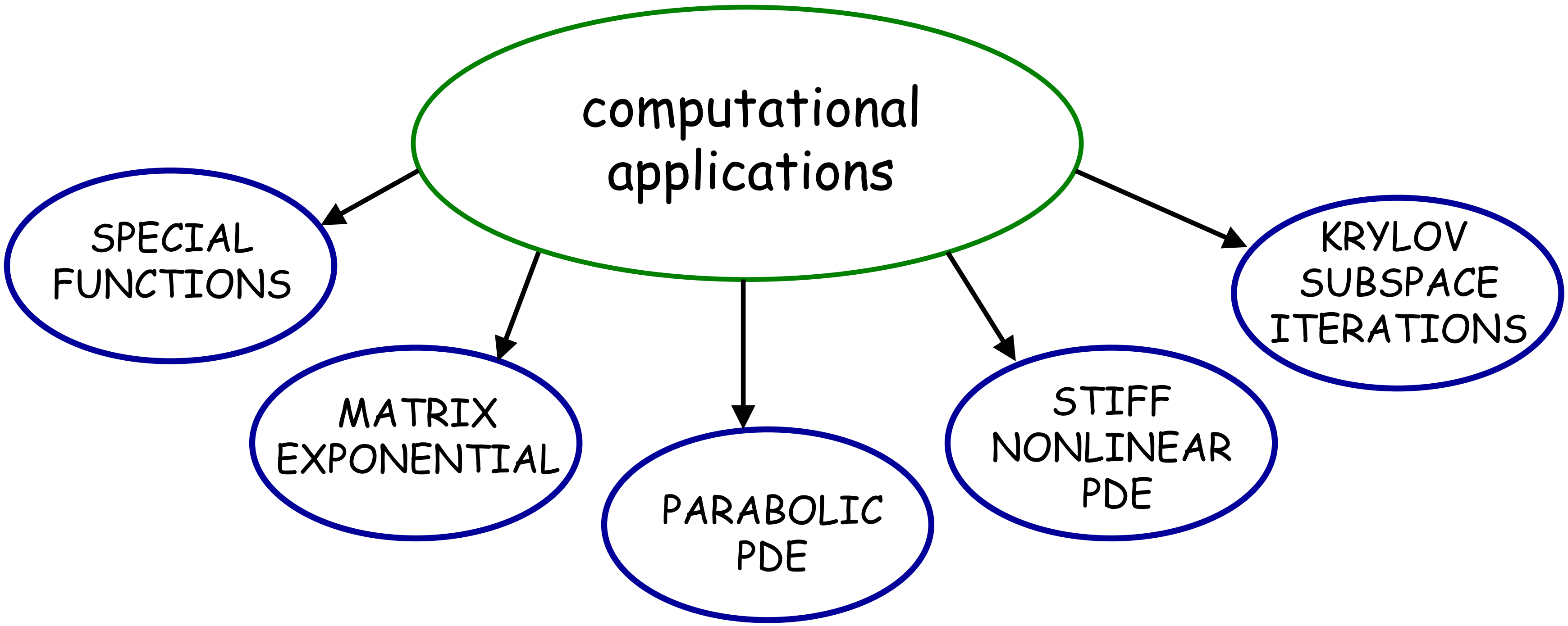
(1) Deform C to contour Γ

(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 $r(z)$

EXAMPLES

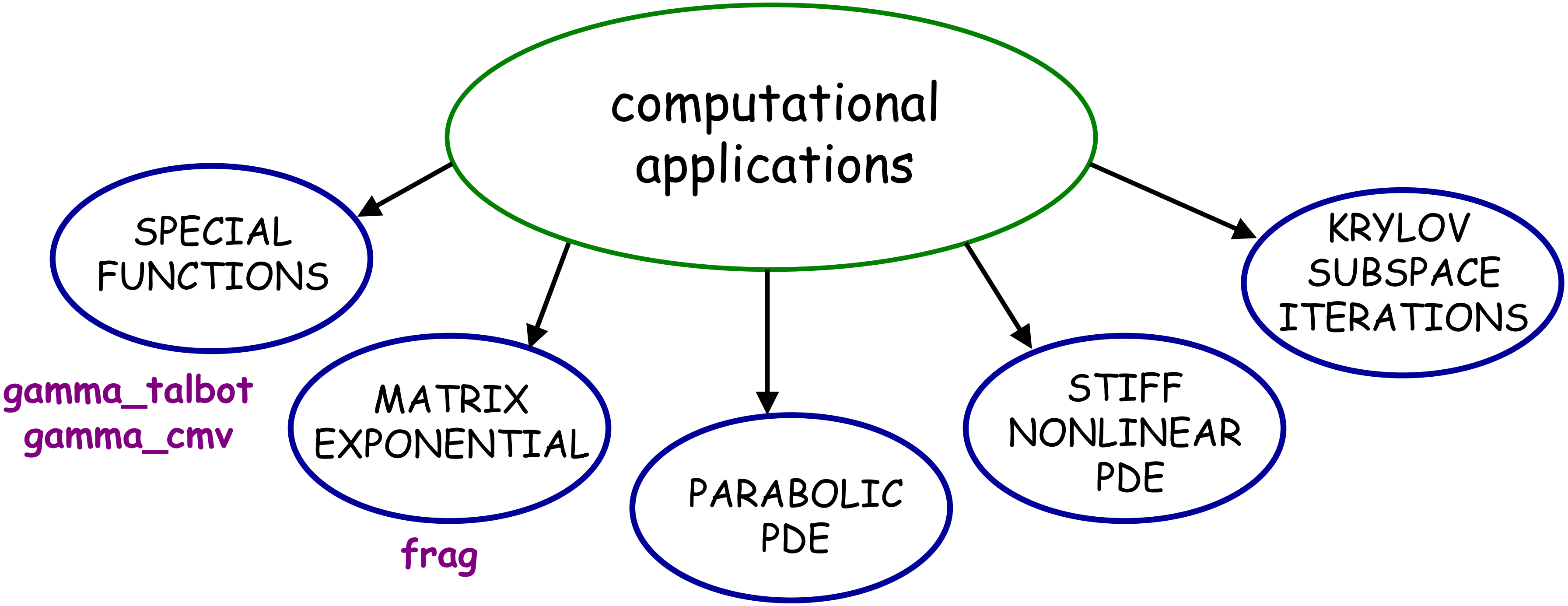
Recall:



Here are some references for these five applications:

	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 05
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

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


computational applications
SPECIAL FUNCTIONS
gamma_talbot
gamma_cmv
MATRIX EXPONENTIAL
frag
PARABOLIC PDE
STIFF NONLINEAR PDE
KRYLOV SUBSPACE ITERATIONS

IN CONCLUSION

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

But they are still the basis of some of the most powerful algorithms.