Ten things you should know about quadrature

Nick Trefethen, March 2016

$$I = \int_{-1}^{1} f(x)dx \qquad I_n = \sum_{k=1}^{n} w_k f(x_k)$$

With thanks to André Weideman for #2, #5, #8, #9
Nick Hale for #4, #5, #7, #8
Nick Higham for #5, #8
Folkmar Bornemann for #6.

A lifetime ago

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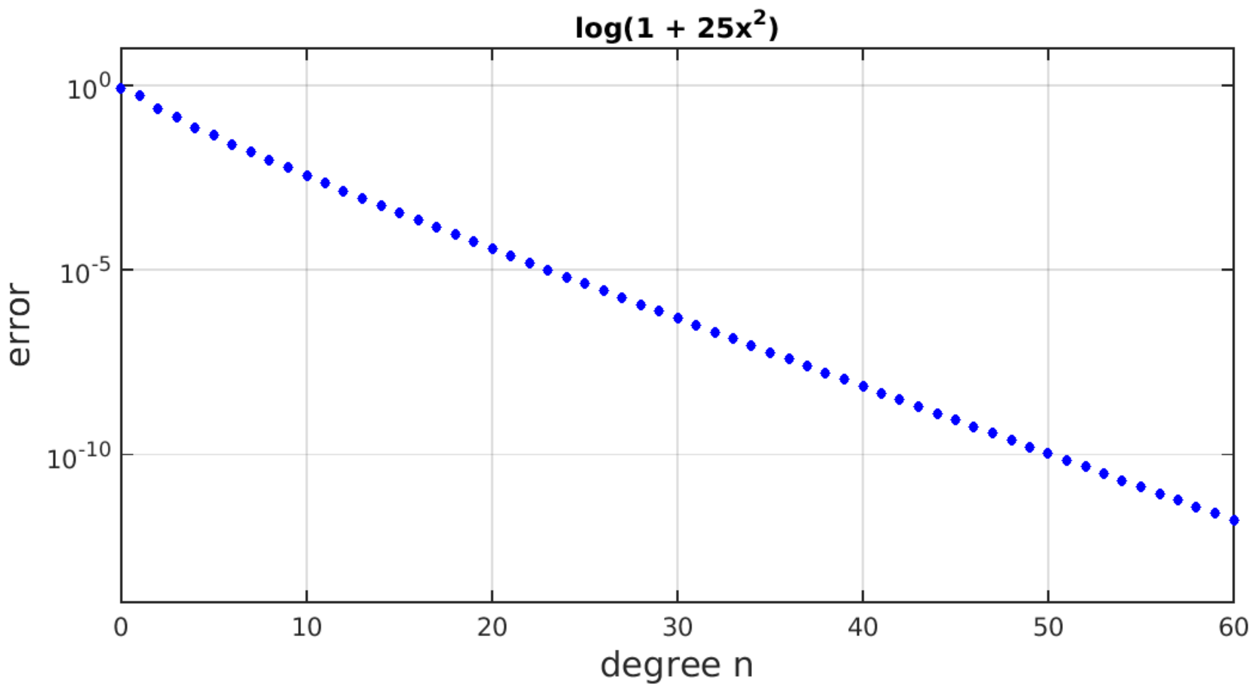
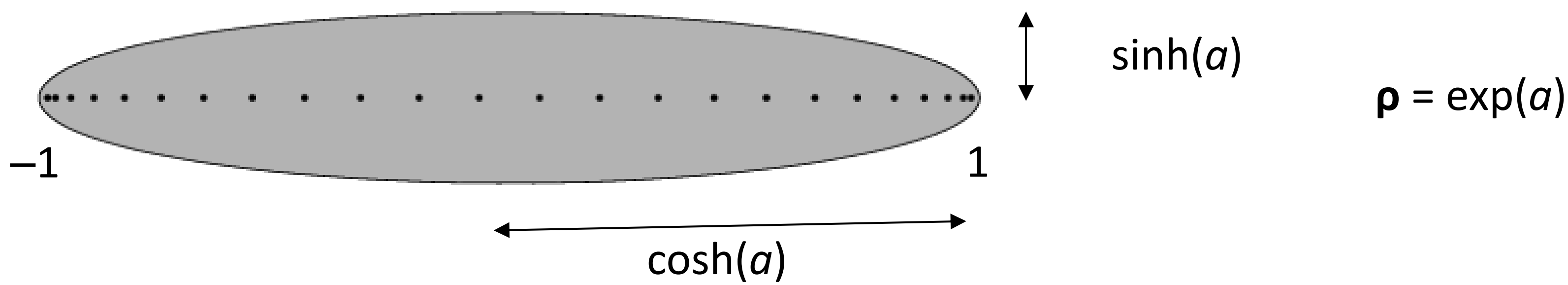
1. Gauss quadrature converges geometrically if the integrand is analytic



19th century result

Explanation

If f is analytic on $[-1,1]$, it is analytic and bounded by M in some Bernstein ρ-ellipse with foci ±1, ρ = semimajor + semiminor axes > 1.



> *Theorem*. The errors in $(n+1)$-point Gauss quadrature satisfy
>
> $$|I - I_n| \leq \frac{5M\rho^{-2n}}{\rho^2 - 1} \quad .$$

Proof. Expand f in a Chebyshev series with coefficients a_k.
By a contour integral one can show (Bernstein 1912):

$$|a_k| \leq 2M\rho^{-k}$$

This implies a bound for the truncated series:

$$|f - f_n| \leq \frac{2M\rho^{-n}}{\rho - 1}$$

which implies for (n+1)-point Gauss quadrature

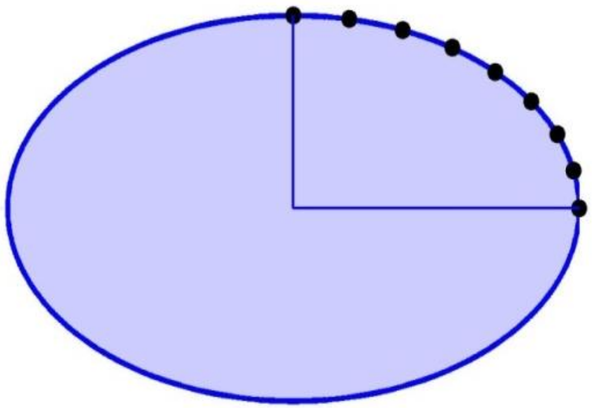
$$|I - I_n| \leq \frac{5M\rho^{-2n}}{\rho^2 - 1}$$

since Gauss is exact for polynomials of degree 2n+1. *QED.*

2. So does the equispaced trapezoidal rule if the integrand is also periodic

See T. + Weideman, *SIAM Review* 2014

Poisson's example: perimeter of ellipse with axes $1/2\pi$ and $0.8/2\pi$:



$$I = (2\pi)^{-1}\int_0^{2\pi} (1 - 0.36\sin^2\theta)^{1/2}\, d\theta$$

Take advantage of 4-fold symmetry.

2 points: **0.9000000000**

3 points: **0.9027692569**

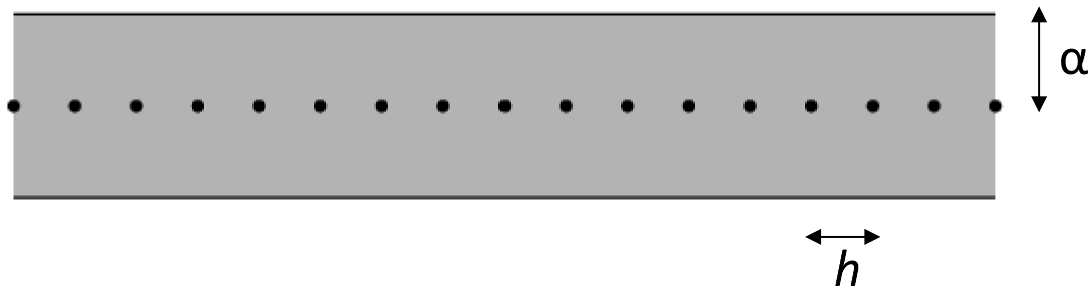
5 points: **0.9027798586**

9 points: **0.9027799272**

"La valeur approchée de I sera I = 0,9927799272."

Poisson 1823

Suppose f is analytic, bounded, and periodic in $S_\alpha = \{z: -\alpha < \operatorname{Im} z < \alpha\}$.



Theorem. The error in trapezoidal rule quadrature is $O(e^{-2\pi\alpha/h})$.

Proof by contour integrals, or by Fourier series and aliasing (with Fourier coefficients estimated by contour integrals).

Davis 1959. He calls the result "folklore".

Analogous result for trapezoidal rule on the real line

Suppose f is analytic and bounded in $S_\alpha = \{z : -\alpha < \mathrm{Im}\, z < \alpha\}$ but not necessarily periodic. Now we use an infinite grid.

Same convergence result as before, under mild assumptions:

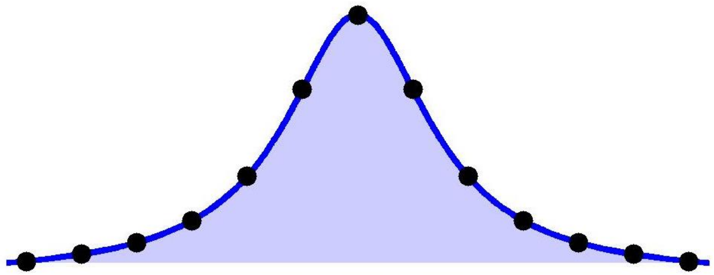
Error in trap. rule quadrature: $O(e^{-2\pi\alpha/h})$

Aitken 1939	Estimating statistical moments
Turing 1943	Application to Riemann zeta function
Goodwin 1949	"It is well known to computers that..."
Faddeeva 1954	Applications to special functions
Fettis 1955	Like Goodwin, assumes $O(e^{-x^2})$ decay
Moran 1958	Connections with probability
McNamee 1964	More general analysis using contour integrals
Martensen 1968	Contour integrals again
Schwartz 1969	Special functions

Example — Runge function

$$I = \pi^{-1}\int_{-\infty}^{\infty}(1+x^2)^{-1}\,\mathrm{d}x$$

$h = \pi$:	1.31303527
$h = \pi/2$:	1.03731468
$h = \pi/3$:	1.00496976
$h = \pi/4$:	1.00067107
$h = \pi/5$:	1.00009070

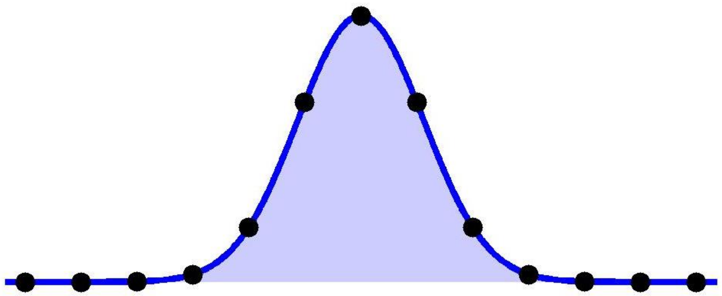


If $h = \pi/n$, error = $O(e^{-2n})$

Example — Gaussian

$$I = \pi^{-1/2}\int_{-\infty}^{\infty}\exp(-x^2)\,\mathrm{d}x$$

$h = \pi$:	1.7726372048
$h = \pi/2$:	1.0366315028
$h = \pi/3$:	1.0002468196
$h = \pi/4$:	1.0000002251
$h = \pi/5$:	1.0000000000



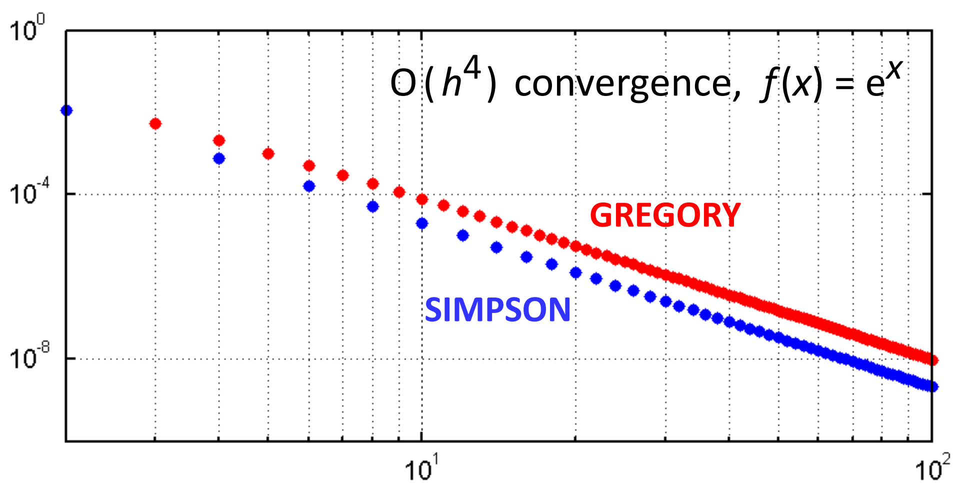
3. Gregory formulas avoid the 2-4-2-4-2 oscillation of Simpson's rule

Euler-Maclaurin: trap. rule + endpoint corrections based on derivatives.

Gregory: same, but endpoint corrections based on finite differences.

Gregory, 1670 (long before Simpson)
See Brass-Petras, *Quadrature Theory,* 2011
and Javed-T., *Numer. Math.* 2016

Composite Simpson's rule:	1/3	4/3	2/3	4/3	2/3	4/3	2/3	...
degree 2 Gregory formula:	3/8	7/6	23/24	1	1	1	1	...



ratio 4.75

4. Gauss nodes and weights can be computed in $O(n)$ operations

Carl Gauss, age 37

"Methodus nova integralium valores per approximationem inveniendi," *Comment. Soc. Reg. Scient. Gotting. Recent.*, 1814

Gene Golub, age 37

"Calculation of Gauss quadrature rules", *Math. Comp.*, 1969 (with J. H. Welsch)

Golub + Welsch 1969: matrix eigenvalue problem. O(n^2) flops.

Golub died in 2007.

O(n) algorithms:

Glaser, Liu + Rokhlin 2007
Bogaert, Michiels + Fostier 2012
Hale + Townsend 2013
Bogaert 2014

(all in *SISC*)

chebfun

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[s,w] = legpts(n)
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5. Every quadrature formula is associated with a rational approximation

$$I = \int_{-1}^{1} f(x)dx \qquad I_n = \sum_{k=1}^{n} w_k f(x_k)$$

I_n is given by a contour integral:

$$I_n = \frac{1}{2\pi i}\int_\Gamma f(z)r(z)dz, \quad r(z) = \sum_{k=1}^{n} \frac{w_k}{z - x_k}$$

(from the Cauchy integral formula)

I is also given by a contour integral:

$$I = \frac{1}{2\pi i}\int_\Gamma f(z)\phi(z)dz, \quad \phi(z) = \log\frac{z+1}{z-1}$$

Proof:

$$f(x) = \frac{1}{2\pi i}\int_\Gamma \frac{f(z)dz}{z-x}, \qquad \int_{-1}^{1}\frac{dx}{z-x} = \log\frac{z+1}{z-1}$$

If $r \approx \phi$ in a region of the z-plane where f is analytic, then $I_n \approx I$.

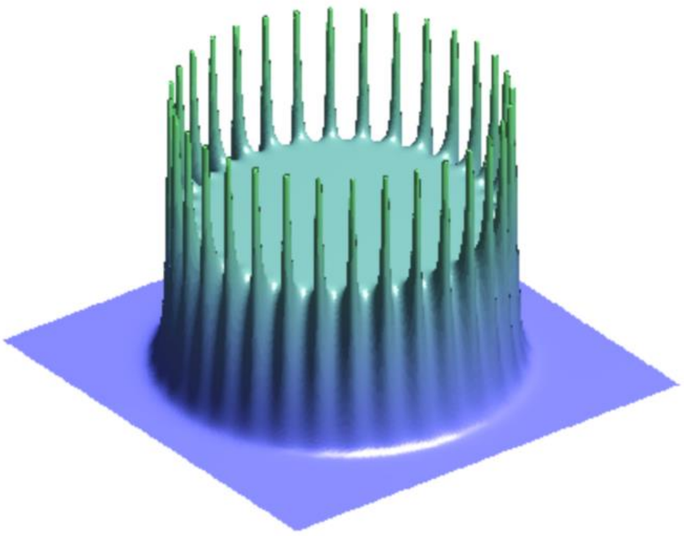
Gauss 1814, Takahasi + Mori 1971

Rational “filter function” from trapezoidal rule on unit circle

$r(z) = (1-z^n)^{-1}$

The simplest example of a rational approximation.

Exponentially close to 1 inside the unit disk and to 0 outside.



$|r(z)|$, $n = 32$

Austin, Kravanja + T., *SINUM* 2015

Approximation → quadrature

Their approximations tell us about accuracy of quadrature formulas (Takahasi + Mori 1971). (See next item, Gauss vs. Clenshaw-Curtis.)

Masatake Mori

Quadrature → approximation

Conversely, quadrature formulas give us rational approximations.

$|x|$ and $\sqrt{x}$: Zolotarev 1877, Stenger 1986, Hale-Higham-T. 2008

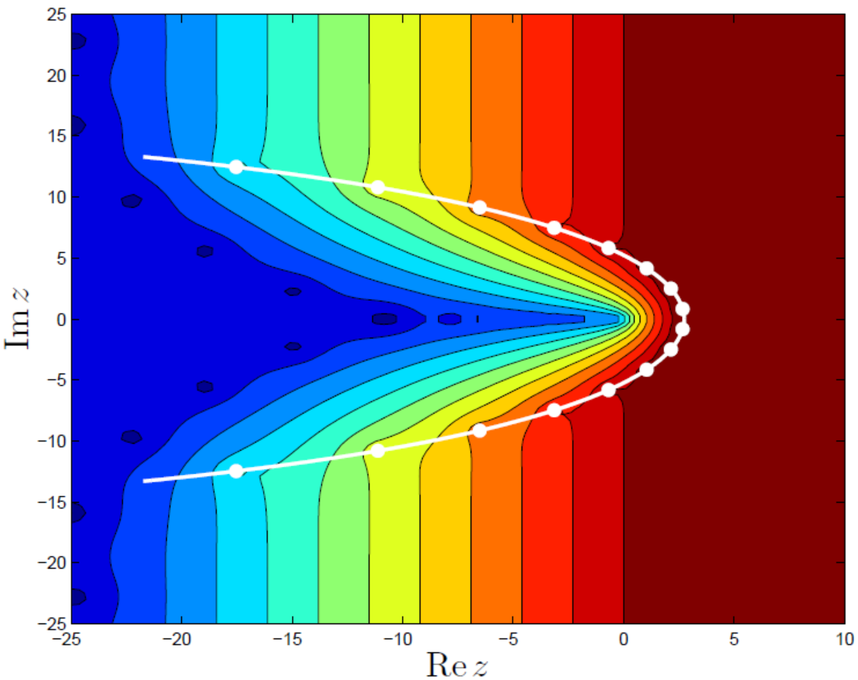
e^x on negative real axis : T.-Weideman-Schmelzer 2006

See chap. 25 of *ATAP.*

Type (16,16) rational approximations of e^x on $(-\infty,0]$

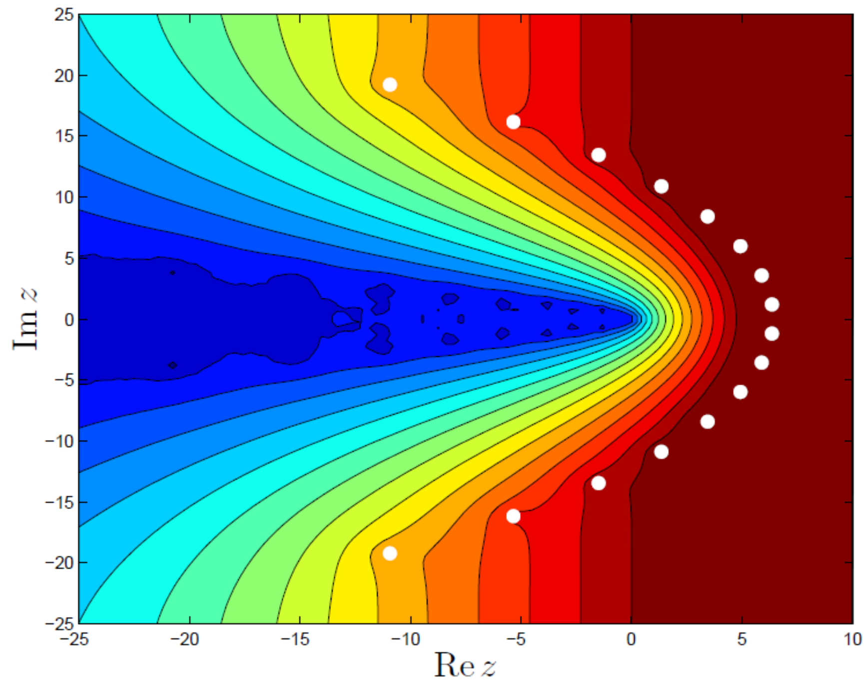
Quadrature on a Hankel contour

(Butcher, Talbot, Weideman,...)



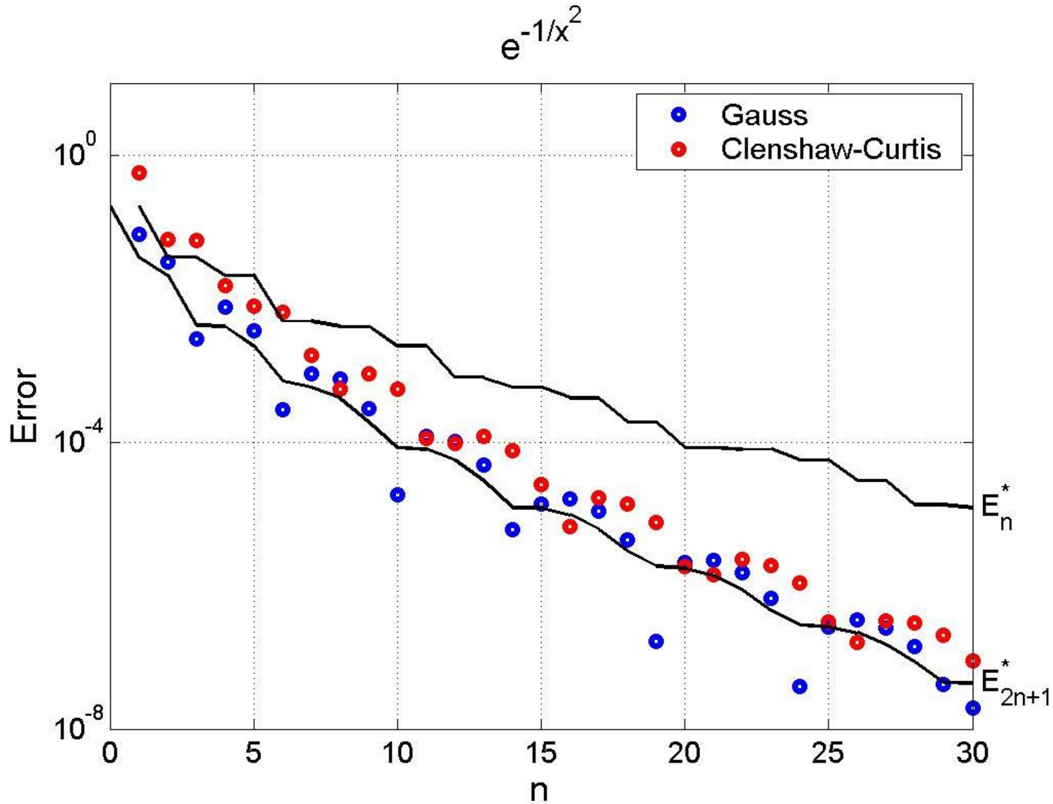
Best approximation

(Cody-Meinardus-Varga,
Gonchar-Rakhmanov, ...)



Contours show errors $|e^z - r_n(z)| = 10^0, 10^{-1},\ldots,10^{-14}$, $n = 16$.
The white dots are the poles of r_n = quadrature points.

6. Clenshaw-Curtis converges as fast as Gauss if the integrand is nonanalytic

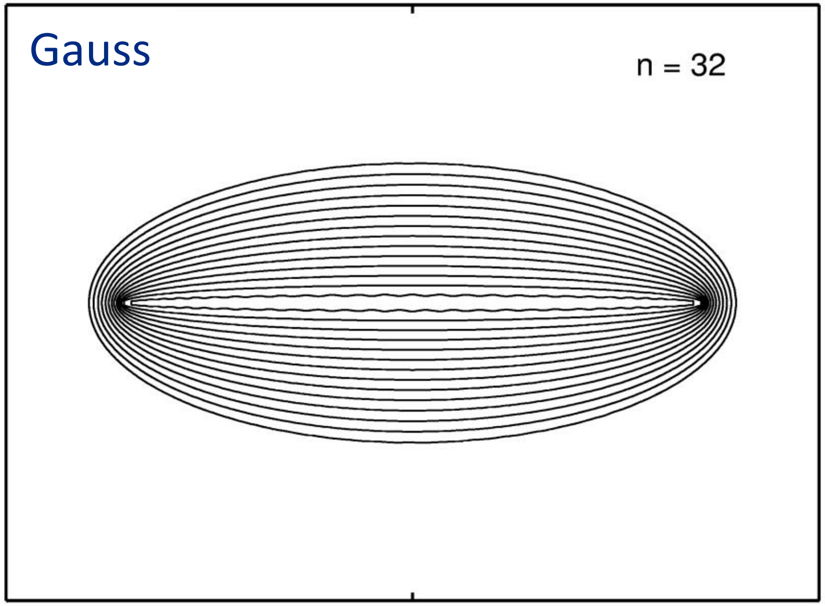


O'Hara + Smith, *Computer J.* 1968
T., *SIREV* 2008
Xiang + Bornemann, *SINUM* 2012

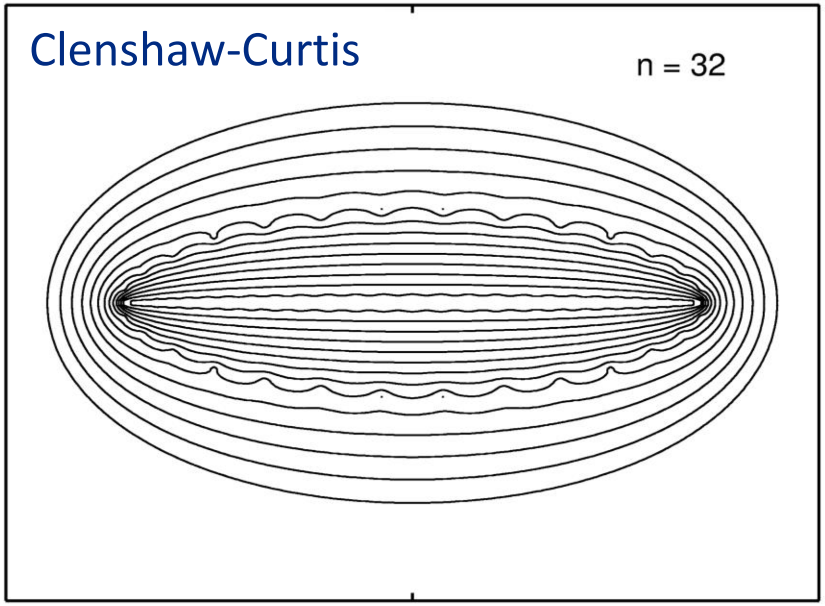
The plots below make it nearly obvious that Clenshaw-Curtis will be as accurate as Gauss for nonanalytic integrands.

The curves are Mori-style error contours for rational approximations

$$| \log((z+1)/(z-1)) - r_n(z) | = 10^0, 10^{-1},\dots,10^{-14} \qquad \text{(from inside out)}$$



$2n+3$ interpolation points, all at ∞



$n-2$ finite interpolation pts, $n+3$ at ∞

Theorem. Let $f^{(k)}$ have bounded variation for some $k \geq 2$.
Then as $n \to \infty$, $|I - I_n| = O(n^{-k-1})$
for both Clenshaw-Curtis and Gauss quadrature.

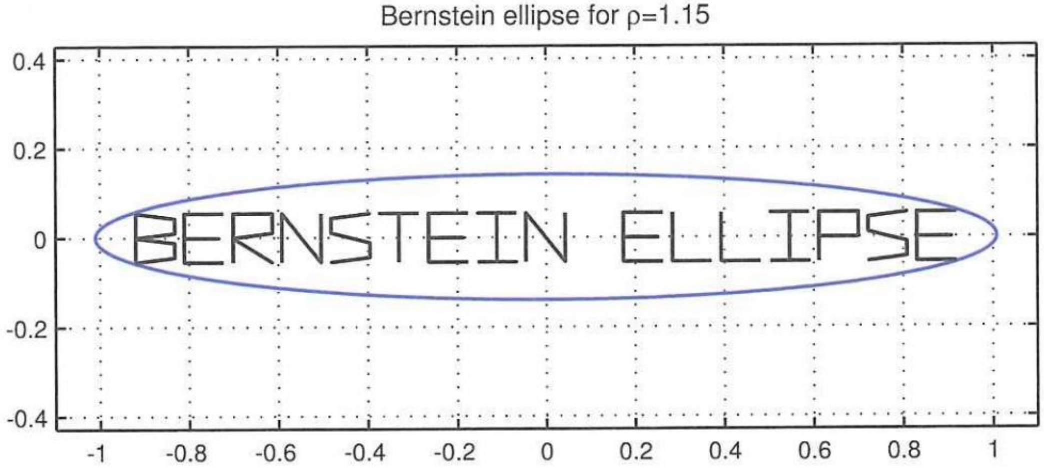
Xiang + Bornemann, *SINUM* 2012

7. All such polynomial-based formulas are suboptimal by a factor of π/2, or $(\pi/2)^d$ in *d* dimensions

Gauss, C-C and other "interpolatory" schemes follow this principle:
(1) interpolate the data by a polynomial, (2) integrate the interpolant.

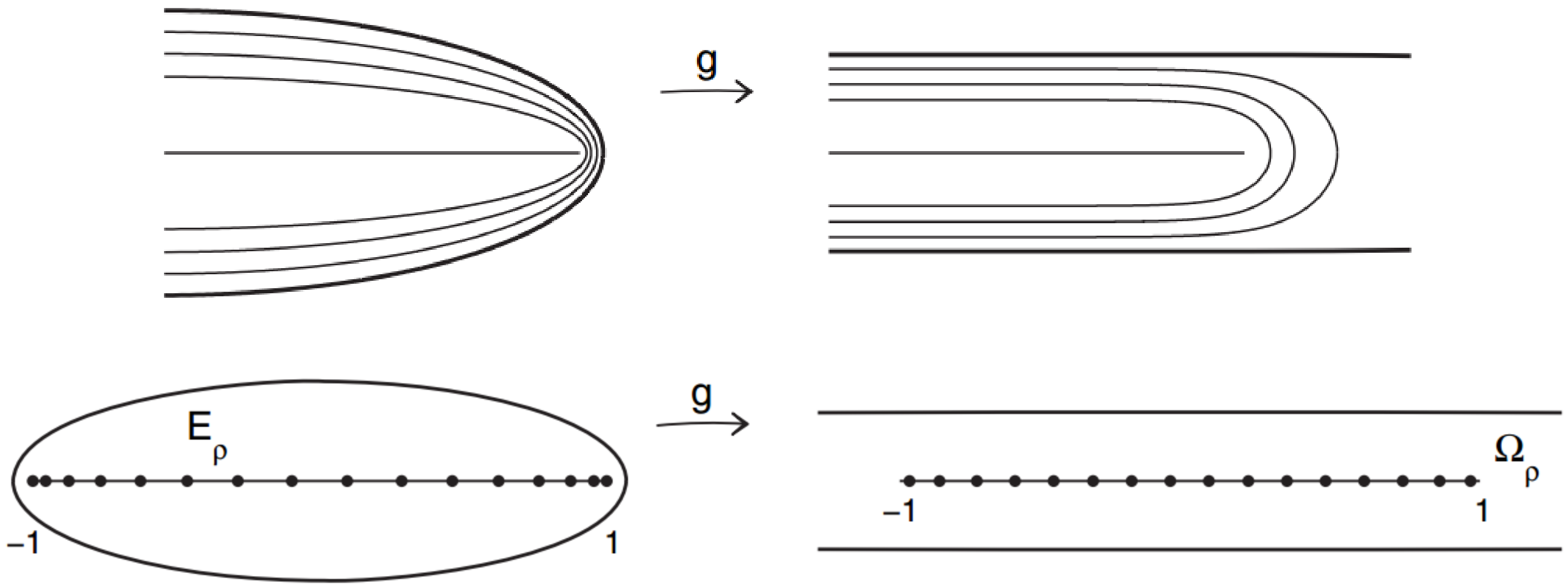
However, the resolution power of polynomials is nonuniform:
outstanding at the endpoints, paying a price in the middle.

This shows up in the shape of a Bernstein ellipse. For f to be analytic here, much more smoothness is required near 0 than near ± 1.



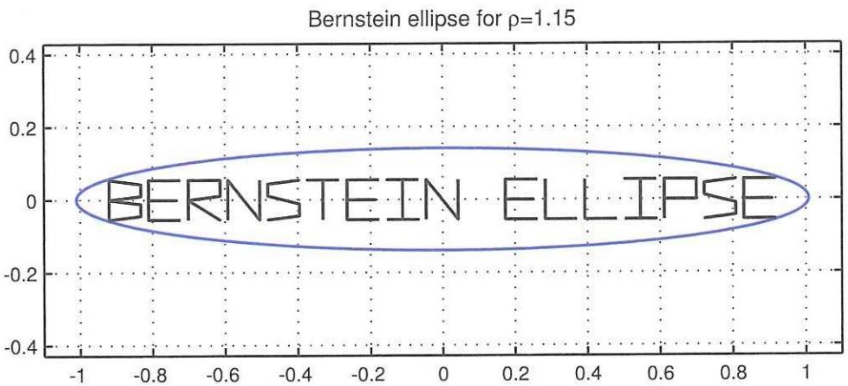
Bakhvalov 1967
Hale + T., *SINUM* 2008

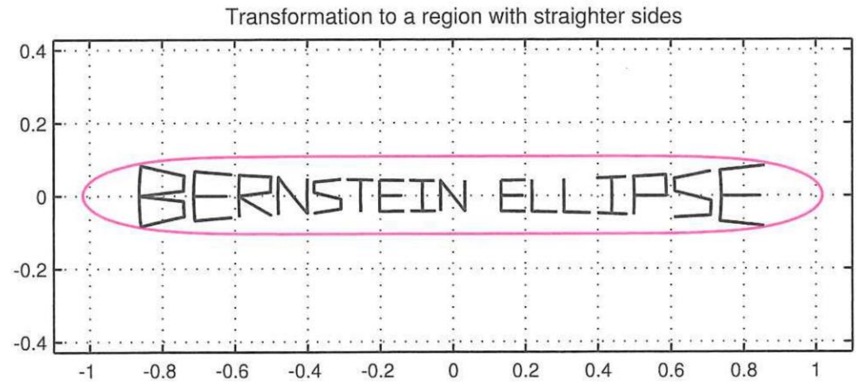
By a conformal map, e.g. from an ellipse to an infinite strip, one can transplant a Gauss or C-C rule to one with more uniform behaviour.



This gives a quadrature rule that corresponds to integration of a nonpolynomial interpolant. Up to π/2 faster convergence for integrands analytic in an ε-neighbourhood of [–1,1].

In d=8 dimensions, improvement by $(\pi/2)^d \approx 37$.





Here is a theorem comparing Gauss with Gauss transplanted by the map from the Bernstein 1.1-ellipse to an infinite strip.

Theorem. Let f be analytic and bounded in the ε-neighbourhood of $[-1,1]$ for some $\varepsilon \le 0.05$. Then

$$\text{Gauss:} \quad |I - I_n| = O(\,(1+\varepsilon)^{-2n}\,)$$

$$\text{Transplanted Gauss:} \quad |I - I_n| = O(\,(1+\varepsilon)^{-3n}\,)$$

8. Quadrature on a Cauchy integral reduces $f(A)$ or eig(A) to $(A-z_kI)^{-1}$

For a matrix or operator A, $f(A)$ is defined by a resolvent integral

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

where C encloses the spectrum of A.

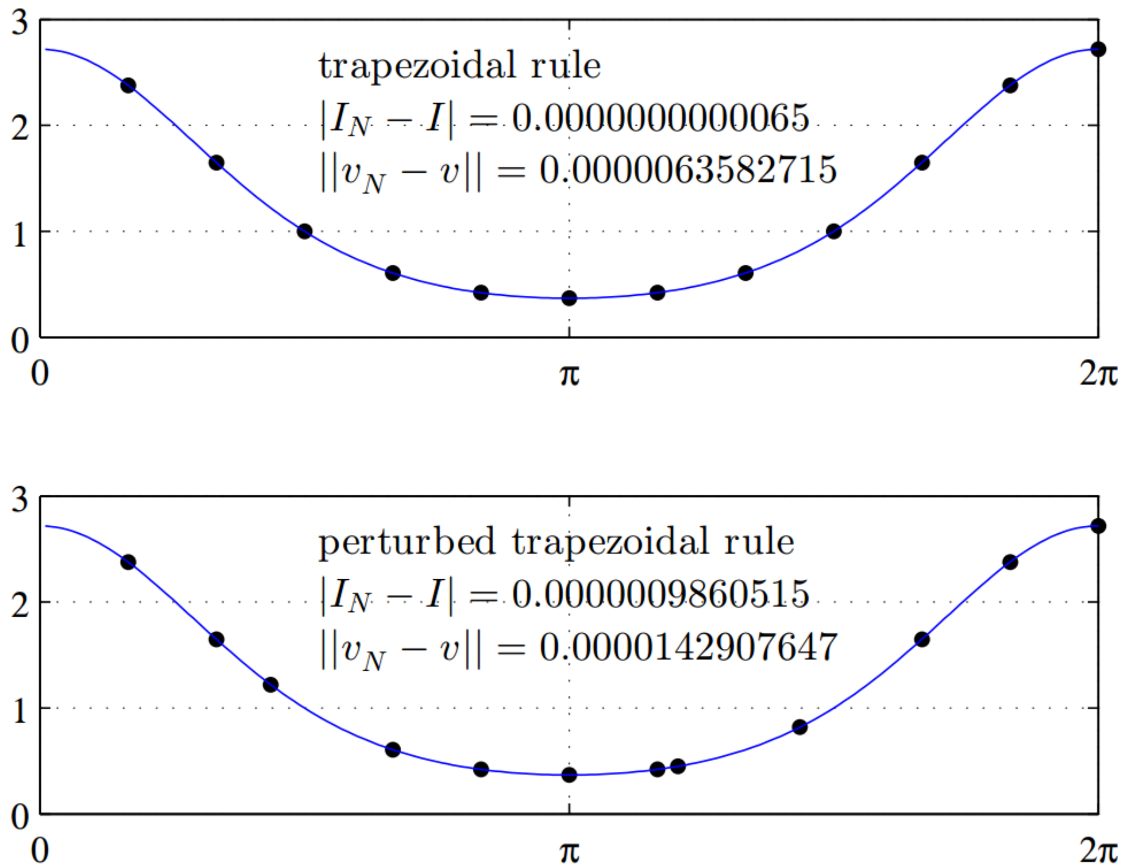
In typical applications 10-20 point quadrature gives full accuracy.
So computing $f(A)$ is reduced to a modest number of linear solves.

T.-Weideman-Schmelzer 2006, Hale-Higham-T. 2008
Lin-Lu-Ying-E 2009, Burrage-Hale-Kay 2012
Lopez-Fernandez-Sauter 2012,….

Other contour integrals find poles of $(z-A)^{-1}$, i.e., eigenvalues *of* A.

Sakurai-Sugiura 2003, Polizzi 2008 (“FEAST”). See Austin-Kravanja-T. 2015

9. #1 and #2 generalize to perturbed points that stay separated (despite the Kadec ¼ theorem)



See T. + Weideman, *SIAM Review* 2014, sec. 9

For Gauss, Clenshaw-Curtis, or periodic trapezoidal rule —

(1) f analytic $\Rightarrow$ $I - I_n = O(C^{-n})$, $C > 1$.

(2) f continuous $\Rightarrow$ $I - I_n \to 0$.

Let $\alpha \geq 0$ be given. Perturb each point up to α times the distance to the next.
(For $\alpha < ½$ the points remain separate; for $\alpha \geq ½$ they may coalesce.)
What happens to (1) and (2)?

Fejér 1918
Kalmár 1926
Kis 1956
Hlawka 1969

Quadrature literature: we know none.
Approximation theory literature: analytic f, no restriction on α.
Sampling theory literature: $\alpha < ¼$ required for a Riesz basis.

Kadec 1964

Theorem (in progress).

(1) holds for all α.

(2) holds iff $\alpha < ½$.

Follows from the approximation theory results.

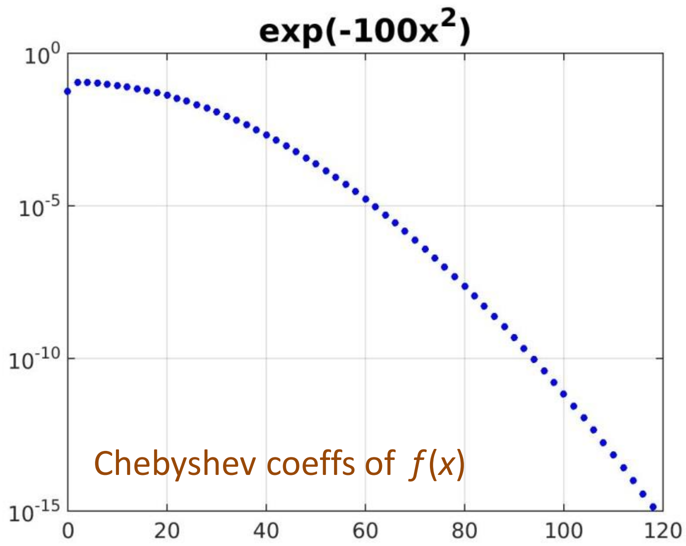
Follows from Pólya's theory of 1933
+ bounds on quadrature weights.

10. Interpolatory cubature is isotropic, but the hypercube is far from isotropic

- Many methods for high-dimensional quadrature/approximation/PDE claim to combat the curse of dimensionality. We have Smolyak cubature, hierarchical bases, sparse grids, interpolatory cubature, Padua points, quasi-Monte Carlo, low-rank compression, tensor trains,….
- Such methods are certainly successful in some applications.
- For "arbitrary" functions f, the curse cannot be beaten. So these methods rely on exploiting special properties of f : often some kind of alignment with axes — anisotropy.
- Authors rarely talk about anisotropy. Some say their methods apply to "smooth" functions — but then define smoothness anisotropically, typically via mixed derivatives.
- Could matters of anisotropy be confronted more squarely?
- Analogy: Krylov matrix iterations are no good for arbitrary matrices; they depend on favourable spectral properties. So the name of the game is preconditioners. Everybody knows this and discusses it squarely.

Surprisingly pronounced anisotropy of the hypercube $[-1,1]^d$

$f(x) = \exp(-100x^2)$ can be resolved to 15 digits on $[-1,1]$ by $p(x)$ of degree 120.



Contour plot of Chebyshev coeffs of $f(x,y)$

What degree $p(x,y)$ is needed for $f(x,y) = \exp(-100(x^2+y^2))$ on $[-1,1]^2$?

Hint: f is isotropic, and multivariate polynomials are isotropic.

Wrong! Need degree $120\sqrt{2}$, not 120, to get 15 digits in the unit square.

In d=8 dimensions, 639 times as many coeffs are needed as you might expect.