Enhancing the trapezoidal rule in the complex plane and along the real axis

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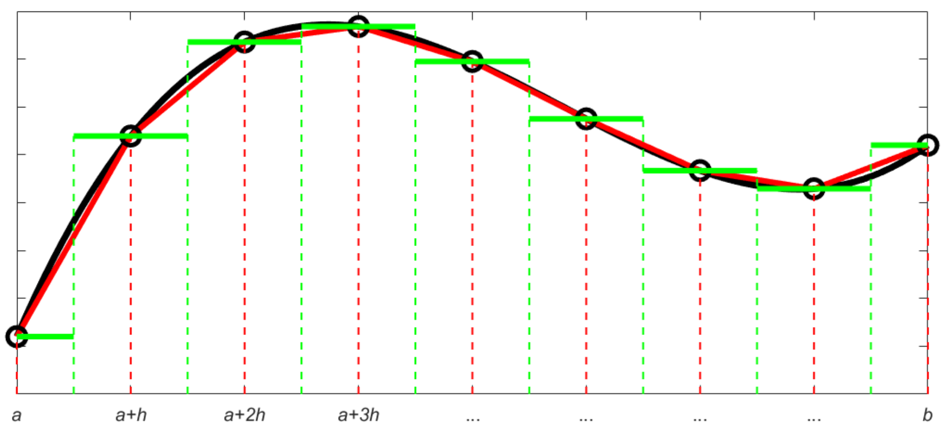
The Trapezoidal Rule (TR)



Function to integrate
Trapezoidal approximation
Equivalent approximation

Used by Babylonian astronomers about 50 BC to calculate Jupiter's position from areas in time-velocity graphs

The **Euler-Maclaurin formula** (1735) for the TR error in semi-infinite case:

$$\int_a^\infty f(x)dx - TR \approx \left\{ \frac{h^2}{12} f^{(1)}(a) - \frac{h^4}{720} f^{(3)}(a) + \frac{h^6}{30240} f^{(5)}(a) - \frac{h^8}{1209600} f^{(7)}(a) + - \ldots \right\}$$

For finite interval [*a*,*b*] (instead of [*a*,∞])

$$\int_a^b f(x)dx - TR \approx \left\{ \frac{h^2}{12} f^{(1)}(a) - \frac{h^4}{720} f^{(3)}(a) + \frac{h^6}{30240} f^{(5)}(a) - + \ldots \right\}$$

$$- \left\{ \frac{h^2}{12} f^{(1)}(b) - \frac{h^4}{720} f^{(3)}(b) + \frac{h^6}{30240} f^{(5)}(b) - + \ldots \right\}$$

The ends of the interval is the by far dominant error source (Gregory 1670)

The Euler-Maclaurin formula (for approximating infinite sums)

$$\int_a^\infty f(x)dx - TR \approx \frac{h^2}{12} f^{(1)}(a) - \frac{h^4}{720} f^{(3)}(a) + \frac{h^6}{30240} f^{(5)}(a) - \frac{h^8}{1209600} f^{(7)}(a) + - \ldots = \sum_{k=2}^{\infty} \frac{B_k}{k!} h^k f^{(k-1)}(a)$$

The **Bernoulli numbers** B_k are defined by $\frac{z}{e^z - 1} = \sum_{k=0}^{\infty} \frac{B_k}{k!} z^k$

$$B_0 = 1,\quad B_1 = -\frac{1}{2},\quad B_2 = \frac{1}{6},\quad B_3 = 0,\quad B_4 = -\frac{1}{30},\quad B_5 = 0,\quad B_6 = \frac{1}{42},\quad B_7 = 0,\quad B_8 = -\frac{1}{30},\quad B_9 = 0,\quad B_{10} = \frac{5}{66},\quad \ldots$$

James Stirling

1692-1770

Colin Maclaurin

1698-1746

Leonhard Euler

1707-1783

The Abel-Plana formulas

Euler-Maclaurin (1735):

$$\int_a^\infty f(x)dx - TR \approx \sum_{k=2}^{\infty} \frac{B_k}{k!} h^k f^{(k-1)}(a)$$

Abel-Plana (1823, 1820):

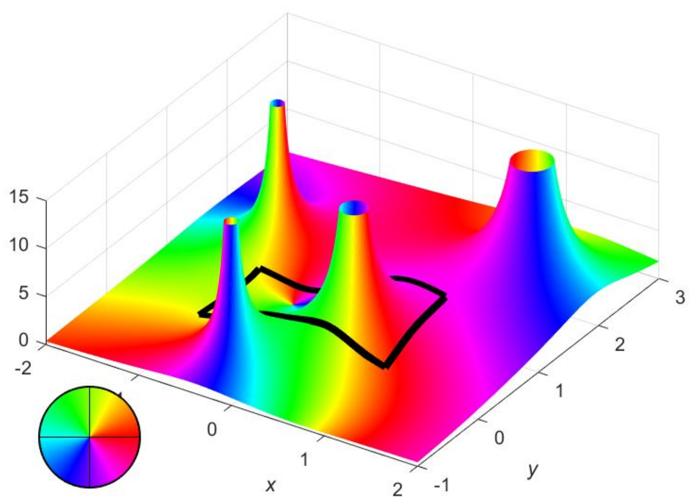
$$\int_a^\infty f(x)dx - TR = -i \int_0^\infty \frac{f(a+it) - f(a-it)}{e^{2\pi t} - 1} dt$$

$$\sum_{k=n}^{\infty} (-1)^n f(k) = (-1)^n \left\{ \frac{1}{2} f(n) + i \int_0^\infty \frac{f(n+it) - f(n-it)}{2\sinh(\pi t)} dt \right\}$$

Amedeo Plana
1781-1864

Niels Henrik Abel
1802-1829

Case 1: Numerical contour integration in the complex plane



Magnitude and phase angle

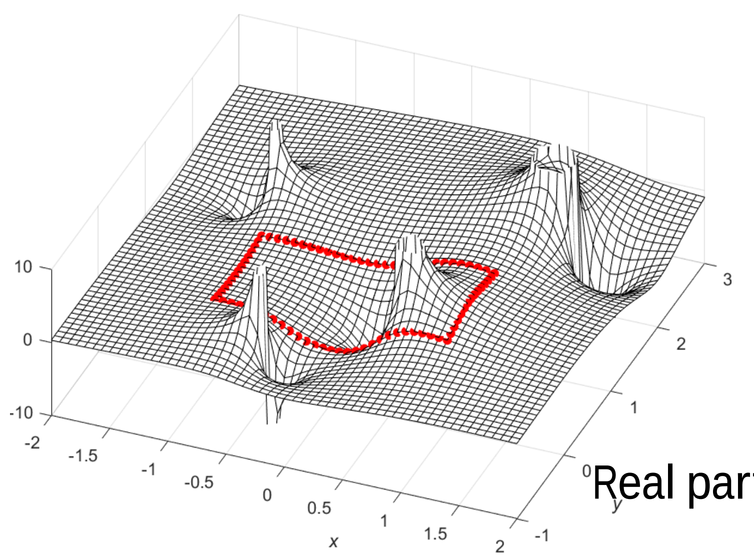
Function illustrated:

$$f(z) = \frac{2}{z-0.4(1+i)} - \frac{1}{z+0.4(1+i)} + \frac{1}{z+1.2-1.6i} - \frac{3}{z-1.3-2i}$$

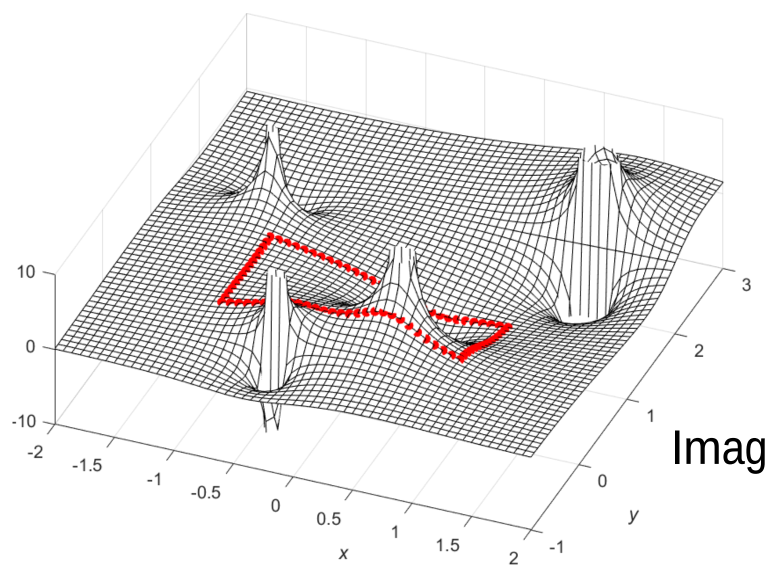
Contours can be open or closed
Follow either Cartesian or hexagonal grid lines

Using only weights at grid points, one can reach accuracy orders $O(h^{50})$ (or even higher).

Grid density shown sufficient for error around 10^{-40}



Real part

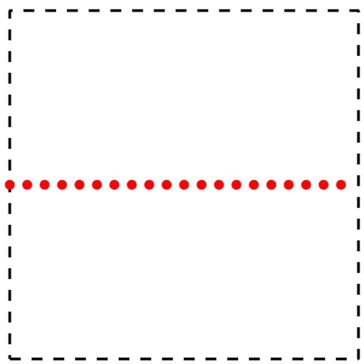


Imaginary part

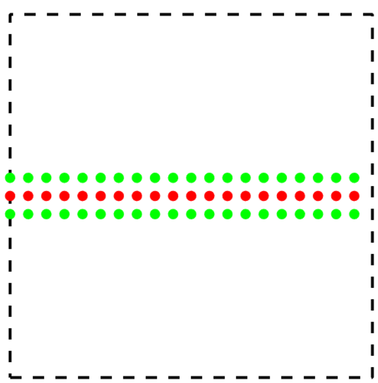
Two main opportunities:

Trapezoidal rule for periodic problem

Standard version



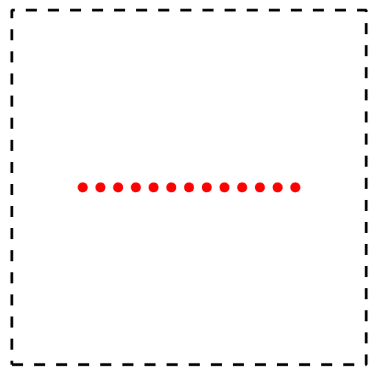
Can one do better?



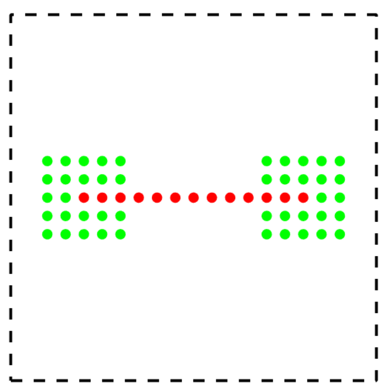
Each pair of lines adds as many correct digits as present in regular TR

Trapezoidal rule for finite interval

Standard version

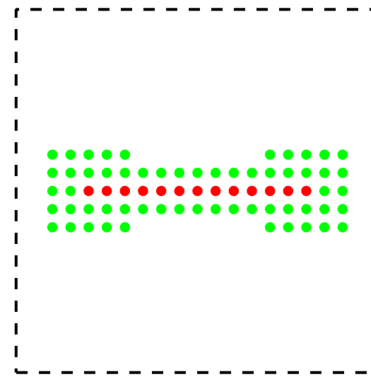


Can one do better?



Order of accuracy one more than number of end correction entries

Combine the two ideas for very accurate integration along finite line sections



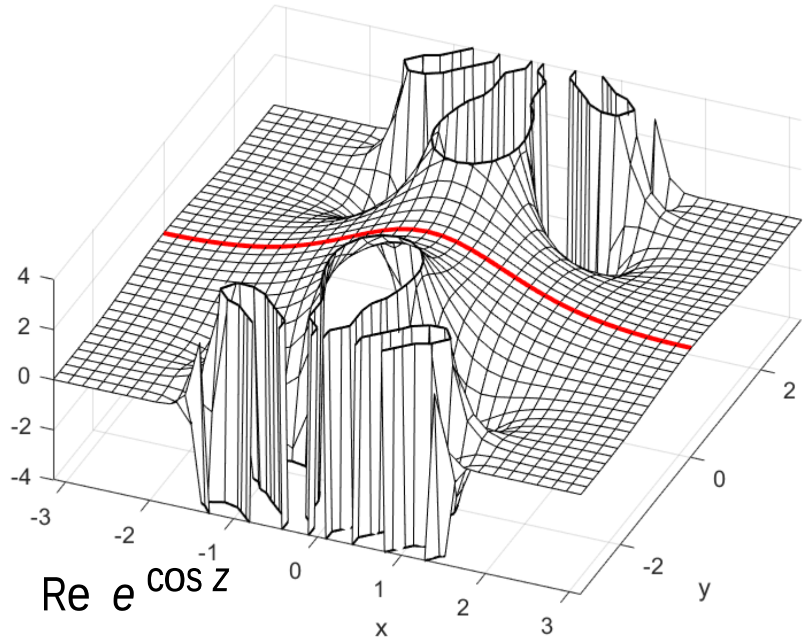
All required weights can be obtained very easily (5 lines in Mathematica)

Periodic function:

Example: $f(z) = e^{\cos z}$

$$\int_{-\pi}^{\pi} e^{\cos x} dx = 2\pi I_0(1) \approx 7.9549265210$$

Fourier series: $f(z) = \sum_{k=-\infty}^{\infty} c_k e^{ikx}$



Aliasing: With N nodes in the period, all modes $k + n \cdot N, n$ integer, are identical at the node points

On the grid, these modes cannot be distinguished (in terms of function values).

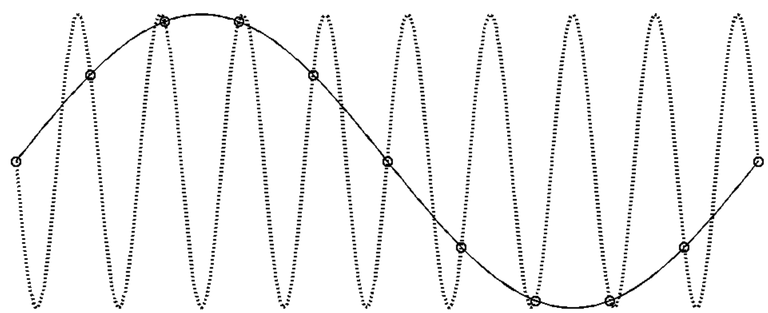


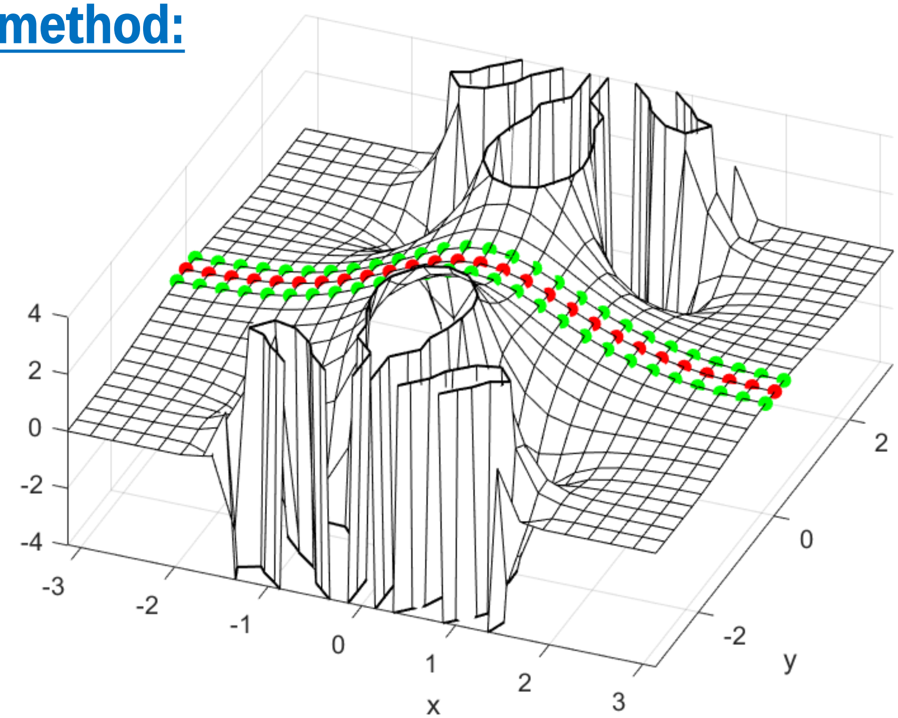
Illustration of aliasing; $N = 10$; $[-\pi, \pi]$
sin(-1x) and sin(9x) same at node points

Periodic example continued, and general method:

$$f(z) = \sum_{k=-\infty}^{\infty} c_k e^{ikx}$$

TR along center line:

$$T_0 = 2\pi \left\{ \ldots + c_{-2N} + c_{-N} + c_0 + c_{+N} + c_{+2N} + \ldots \right\}$$



$2\pi c_0$ is the exact integral; other terms are aliasing errors.

Coefficients c_k decay faster than exponentially

TR along lines below and above:

$$T_- = 2\pi \left\{ \ldots + c_{-2N} e^{-4\pi} + c_{-N} e^{-2\pi} + c_0 + c_{+N} e^{2\pi} + c_{+2N} e^{4\pi} + \ldots \right\}$$

$$T_+ = 2\pi \left\{ \ldots + c_{-2N} e^{4\pi} + c_{-N} e^{2\pi} + c_0 + c_{+N} e^{-2\pi} + c_{+2N} e^{-4\pi} + \ldots \right\}$$

These three results can be combined to eliminate the leading errors due to the $c_{\pm N}$ terms

Periodic example continued, and general method:

Combination that eliminates the $c_{\pm N}$ terms:

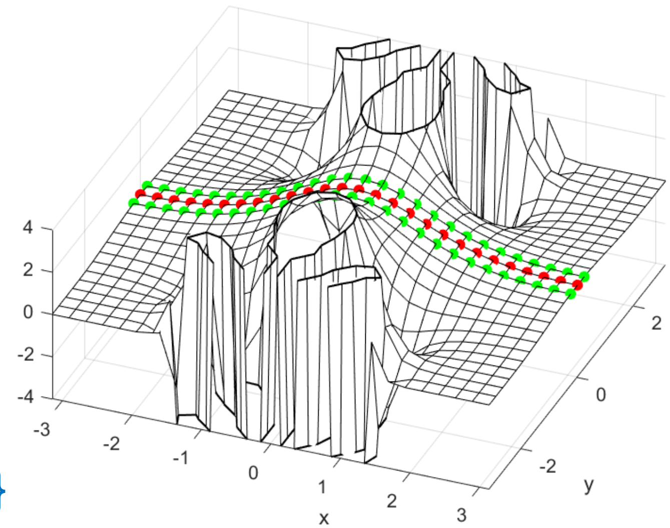
$$T = \frac{1}{(2\sinh\pi)^2}\{-T_- + 2\cosh(2\pi)\,T_0 - T_+\} = 2\pi c_0 + O(c_{\pm 2N})$$

Numerical values for the three coefficients approximately

{ -0.00187, 1.00375, -0.00187 }

If using 5 lines, error $O(c_{\pm 3N})$, coefficients approximately

{ $6.5\cdot10^{-9}$, -0.00188, 1.00376, -0.00188, $6.5\cdot10^{-9}$ }



Same idea equally available on hexagonal grids

Coefficients to use along three center lines

{ 0.00430, 0.99141, 0.00430 }

Along 5 center lines

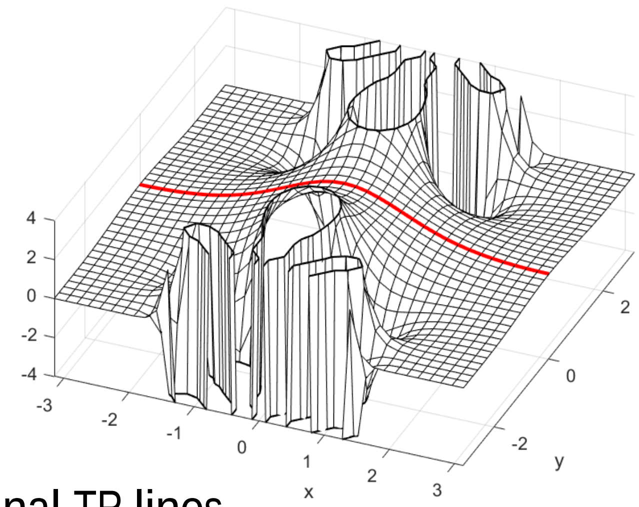
{ $-8.1\cdot10^{-8}$, 0.00428, 0.99144, 0.00428, $-8.1\cdot10^{-8}$}

All multi-line TR formulas can alternatively be derived by contour integration in the complex plane, based on the analytic properties of the function $\pi \cot \pi z$.

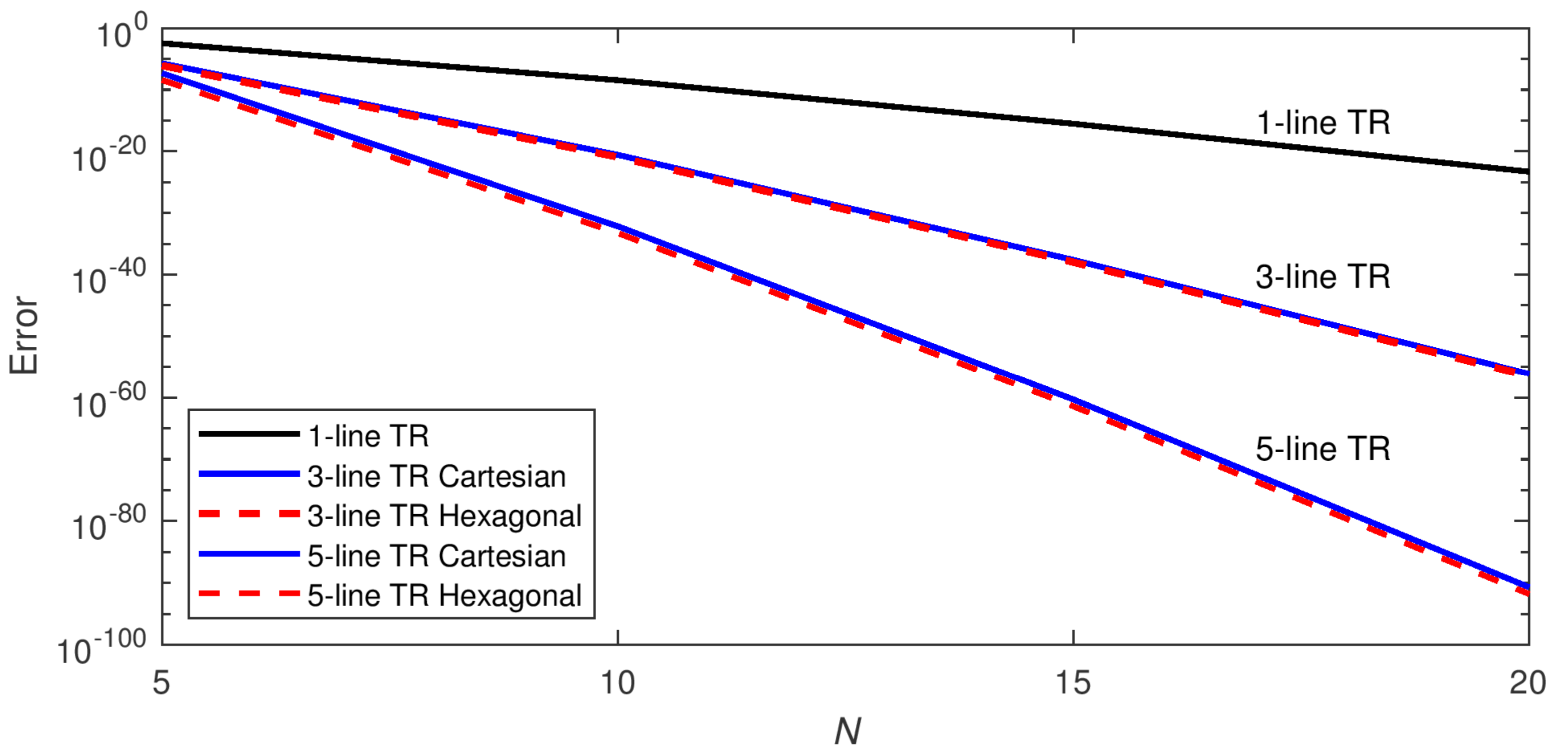
Periodic example continued, and general method:

Test problem ⇨⇨

$$f(z) = e^{\cos z}$$



Log-linear plot – convergence slightly better than spectral.
Number of correct digits increases as expected with additional TR lines.



Trapezoidal rule for finite interval – End corrections:

Weights in regular (1-line) TR at $z = a$ (left end) : $h\left\{\tfrac{1}{2},\quad 1,\quad 1,\quad 1,\quad 1,\quad 1,\ldots\right\}$

Euler-Maclaurin: Error in regular TR on an infinite interval:

$$\int_a^b f(z)\,dz - TR = \left\{\frac{h^2}{12} f^{(1)}(a) - \frac{h^4}{720} f^{(3)}(a) + \frac{h^6}{30240} f^{(5)}(a) - \frac{h^8}{1209600} f^{(7)}(a) + - \ldots\right\}$$

Weights in 3-line TR at $z = a$:

$$h\frac{1}{(2\sinh\pi)^2}\left\{\begin{matrix} [\quad -1 \quad]\cdot\{\tfrac{1}{2}, & 1, & 1, & 1, & 1, & 1, & \ldots\} \\ [2\cosh 2\pi]\cdot\{\tfrac{1}{2}, & 1, & 1, & 1, & 1, & 1, & \ldots\} \\ [\quad -1 \quad]\cdot\{\tfrac{1}{2}, & 1, & 1, & 1, & 1, & 1, & \ldots\} \end{matrix}\right\}$$

Euler-Maclaurin counterpart available – again only odd derivatives but different coefficients.

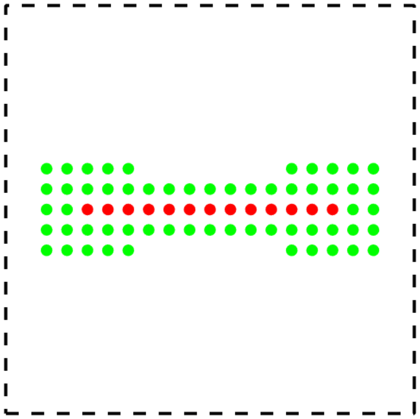
Second key ingredient for end correction: Cauchy's integral formula

$$f^{(k)}(z) = \frac{k!}{2\pi i}\int_\Gamma \frac{f(\xi)}{(\xi - z)^{k+1}}\,d\xi$$

- Exact – no need for path to be very close to z
- Instead of finding quadrature weights around a contour for each derivative, whole EM-type expansion can be approximated by single FD stencil in complex plane

Examples of end correction FD stencil in 3-line TR case:

Left end: 3-line TR: $h\dfrac{1}{(2\sinh\pi)^2}\left\{\begin{array}{l}[\quad -1 \quad]\cdot\{\tfrac{1}{2},\ 1,\ 1,\ 1,\ 1,\ 1,\ \ldots\} \\ [2\cosh 2\pi]\cdot\{\tfrac{1}{2},\ 1,\ 1,\ 1,\ 1,\ 1,\ \ldots\} \\ [\quad -1 \quad]\cdot\{\tfrac{1}{2},\ 1,\ 1,\ 1,\ 1,\ 1,\ \ldots\}\end{array}\right\}$

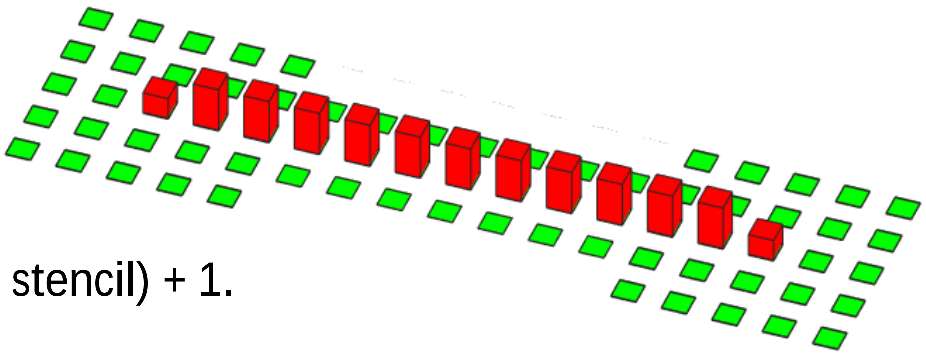


3-line Mathematica code give all end correction weights for any combination of multi-line TR and stencil size.

For 3-line TR and 5x5 stencil:

$-c_8+ic_9$	$-c_{10}+ic_{11}$	ic_{12}	$c_{10}+ic_{11}$	c_8+ic_9
$-c_6+ic_7$	$-c_2+ic_3$	ic_4	c_2+ic_3	c_6+ic_7
$-c_5$	$-c_1$	0	c_1	c_5
$-c_6-ic_7$	$-c_2-ic_3$	$-ic_4$	c_2-ic_3	c_6-ic_7
$-c_8-ic_9$	$-c_{10}-ic_{11}$	$-ic_{12}$	$c_{10}-ic_{11}$	c_8-ic_9

$$\begin{array}{llll} c_1 \approx 0.01584538613124865210, & c_7 \approx -0.00001086091533534879, \\ c_2 \approx 0.00196114131223055449, & c_8 \approx -0.00000017592393798095, \\ c_3 \approx -0.00179604028335645052, & c_9 \approx 0.00000017192139599287, \\ c_4 \approx -0.01936320425382213082, & c_{10} \approx 0.00001143418528633658, \\ c_5 \approx -0.00006132067581641948, & c_{11} \approx -0.00001107294056928483, \\ c_6 \approx 0.00001116130210519658, & c_{12} \approx 0.00006428142367113119. \end{array}$$

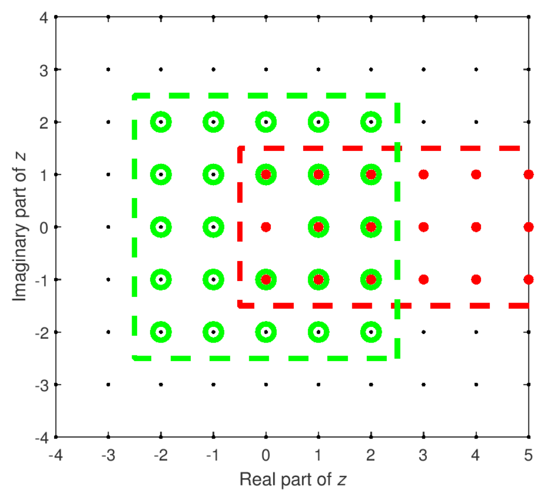


Accuracy $O(h^p)$ where p = (number of nodes in stencil) + 1.

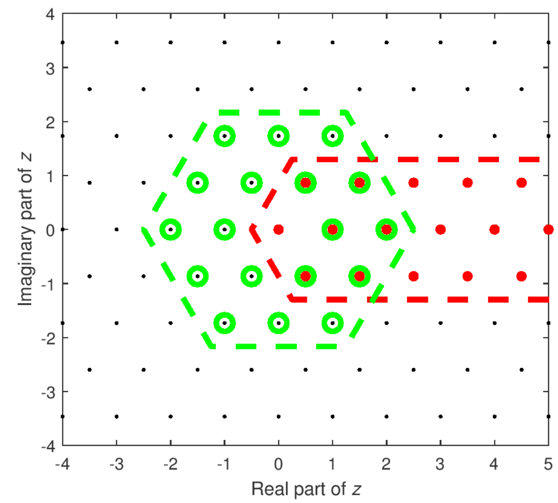
All weights are coefficients times h (step length in any direction in the complex plane)
Weights that are not part of 1-line TR almost vanishingly small.

Examples of end correction FD stencil in 3-line TR case:

Cartesian grid



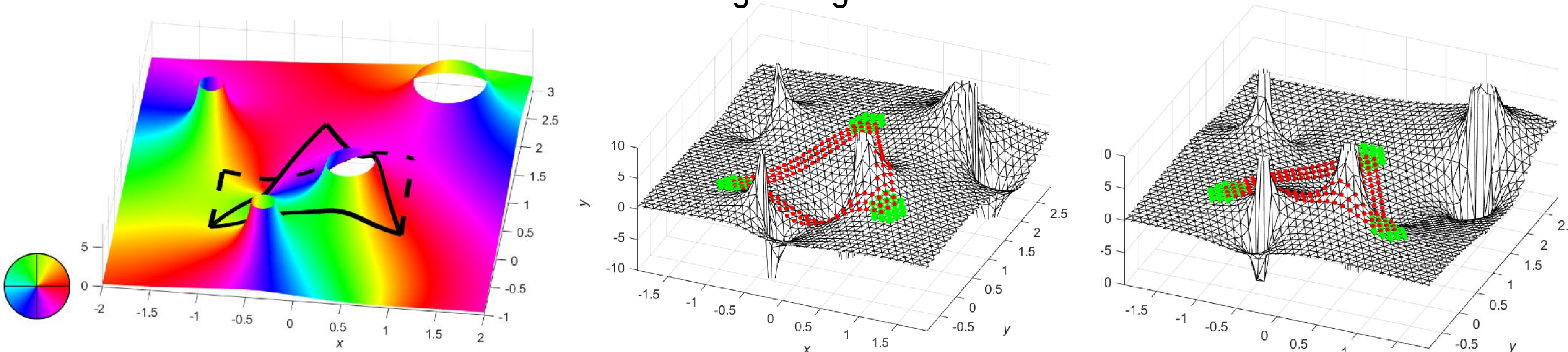
Hexagonal grid



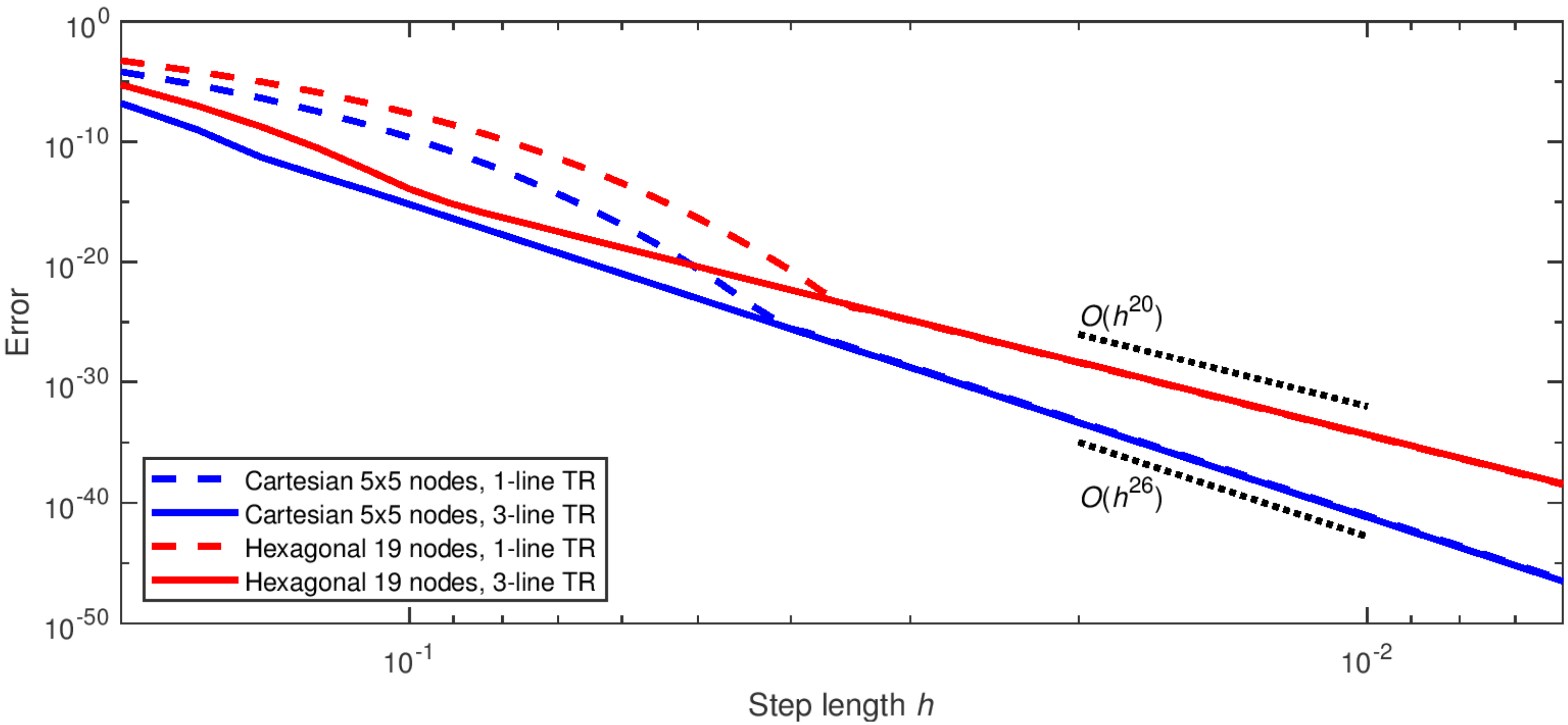
	Cartesian grid	Hexagonal grid
Number of nodes:	5x5 = 25 nodes	19 nodes
Accuracy order:	$O(h^{26})$	$O(h^{20})$
Largest magnitude Off centerline entry:	0.019	0.012

Test problem with closed contours:

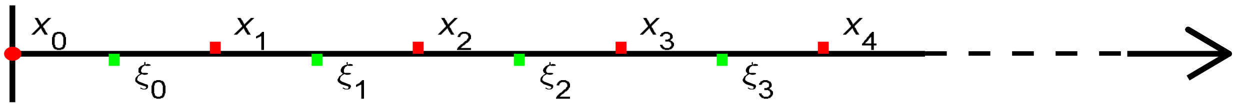
Hexagonal grid with h = 0.1



Magnitude and phase Real part Imaginary part



Case 2: Euler-Maclaurin applied to infinite sums; Midpoint Rule



$$\int_{x_0}^{\infty} f(x)dx - h\sum_{k=0}^{\infty} f(\xi_k) \approx -\frac{h^2}{24} f^{(1)}(x_0) + \frac{7h^4}{5760} f^{(3)}(x_0) - \frac{31h^6}{967680} f^{(5)}(x_0) + \frac{127h^8}{154828800} f^{(7)}(x_0) + - \ldots$$

Define $F(x) = -\int_x^{\infty} f(t)dt$ The EM2 formula then becomes

$$\sum_{k=0}^{\infty} f(k+\tfrac{1}{2}) = -F(0) + \frac{1}{24} F^{(2)}(0) - \frac{7}{5760} F^{(4)}(0) + \frac{31}{96780} F^{(6)}(0) - \frac{127}{154828800} F^{(8)}(0) + \ldots$$

Apply regular cantered FD approximations, step h = ½. Produces table of weights:

	Weights for $F(x)$ at x-locations										
μ	$-\frac{5}{2}$	-2	$-\frac{3}{2}$	-1	$-\frac{1}{2}$	0	$\frac{1}{2}$	1	$\frac{3}{2}$	2	$\frac{5}{2}$
1						-1					
2					$\frac{1}{6}$	$-\frac{4}{3}$	$\frac{1}{6}$				
3				$-\frac{1}{30}$	$\frac{3}{10}$	$-\frac{23}{15}$	$\frac{3}{10}$	$-\frac{1}{30}$			
4			$\frac{1}{140}$	$-\frac{8}{105}$	$\frac{57}{140}$	$-\frac{176}{105}$	$\frac{57}{140}$	$-\frac{8}{105}$	$\frac{1}{140}$		
5		$-\frac{1}{630}$	$\frac{5}{252}$	$-\frac{38}{315}$	$\frac{125}{252}$	$-\frac{563}{315}$	$\frac{125}{252}$	$-\frac{38}{315}$	$\frac{5}{252}$	$-\frac{1}{630}$	
6	$\frac{1}{2772}$	$-\frac{2}{385}$	$\frac{25}{693}$	$-\frac{568}{3465}$	$\frac{1585}{2772}$	$-\frac{6508}{3465}$	$\frac{1585}{2772}$	$-\frac{568}{3465}$	$\frac{25}{693}$	$-\frac{2}{385}$	$\frac{1}{2772}$

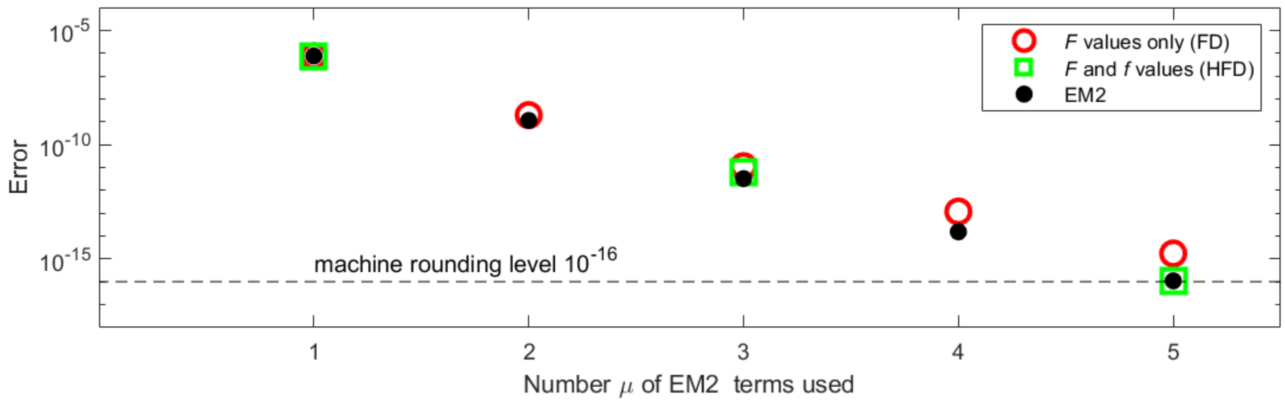
Example

Approximate: $\sum_{k=1}^{\infty} f(k) \approx 0.25903856926239039237$

where
$$f(x) = \frac{x \operatorname{erfinv}\left(\arctan \frac{1}{\sqrt{1+x^2}}\right)}{(x^2+2)\sqrt{1+x^2}}, \quad F(x) = \frac{e^{-\left(\operatorname{erfinv}\left(\arctan \frac{1}{\sqrt{1+x^2}}\right)\right)^2} - 1}{\sqrt{\pi}}$$

To reach error around 10^{-16} by direct summation requires approximately 100,000,000 terms.

Instead, sum directly $\sum_{k=1}^{19} f(x)$ and apply EM2 to $\sum_{k=20}^{\infty} f(x)$.



μ = 5 terms of EM2 requires a total of 9 function evaluations, or evaluation of up through the 7th derivative of *f*(*x*) (EM2).

Case 3: Enhancing the Trapezoidal Rule on a finite interval

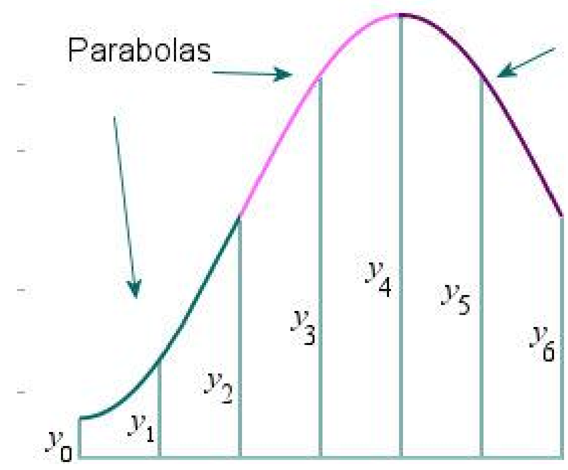
Trapezoidal rule: Fit by piecewise linear functions

Gives weights $h\left[\frac{1}{2}\ 1\ 1\ 1\ 1\ 1\ \ldots\ 1\ \frac{1}{2}\right]$

Simpson's rule: Fit by succession of quadratics

Simpson (1710-1761); however used by Kepler (1571-1630)

Gives weights $\frac{h}{3}[1\ 4\ 2\ 4\ 2\ 4\ 2\ldots\ 4\ 1]$



Newton-Cotes idea: Continue by using piecewise cubics, quartics, etc.

Newton (1642-1726), Cotes (1682-1716)

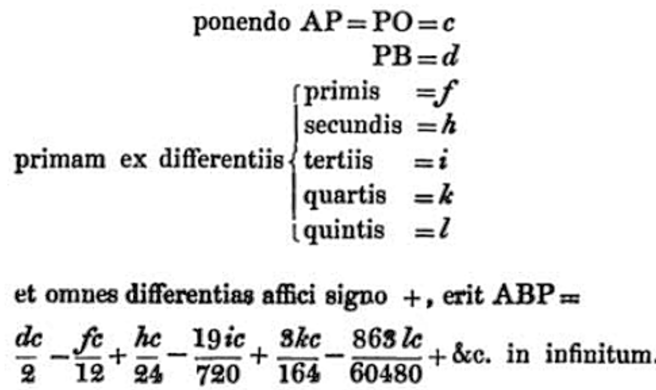
Concept flawed for several reasons:

- Essentially ALL errors in Trap. Rule comes from the ends; should do corrections there and NOT 'contaminate' throughout the whole interior.
- For periodic problem, Trap error ≈ (Simpson error)^2.
- Becomes very unstable for increasing orders.

James Gregory (1638-1675)

Extract from a letter by Gregory to John Collins, November 23, 1670:

Transcribed to print by Oxford Univ. Press, 1840 → → →



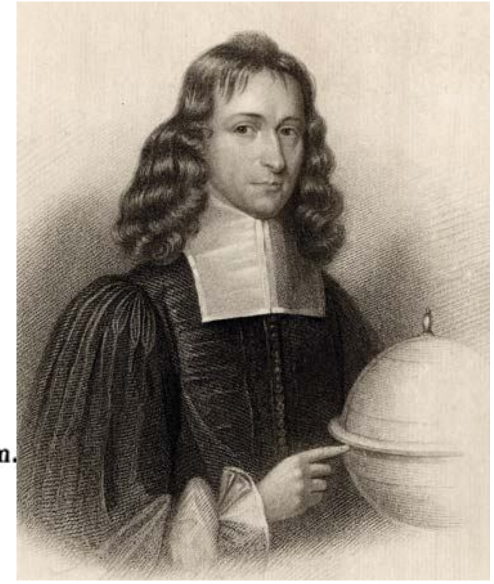
ponendo $AP = PO = c$

$PB = d$

primam ex differentiis $\begin{cases} \text{primis} & = f \\ \text{secundis} & = h \\ \text{tertiis} & = i \\ \text{quartis} & = k \\ \text{quintis} & = l \end{cases}$

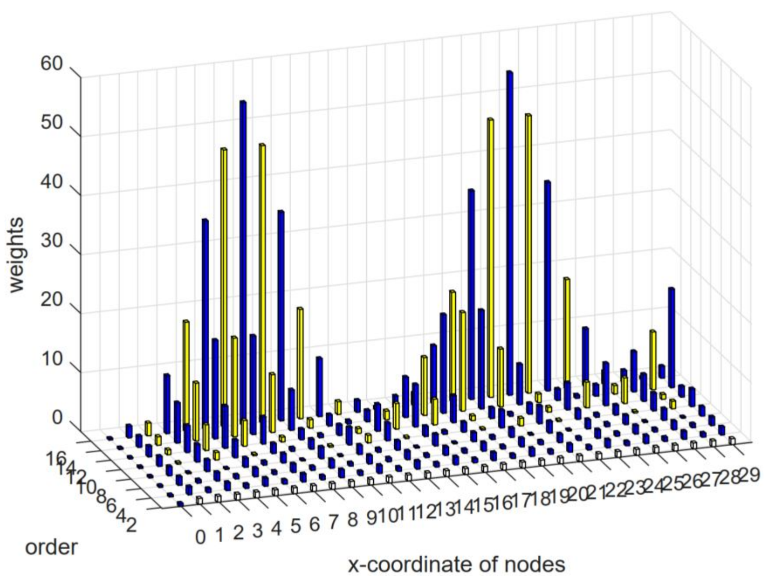
et omnes differentias affici signo $+$, erit $ABP =$

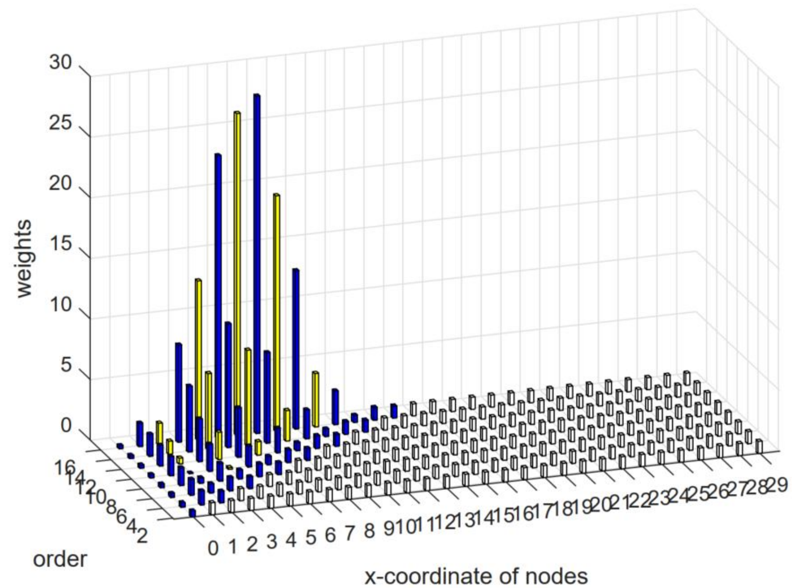
$$\frac{dc}{2} - \frac{fc}{12} + \frac{hc}{24} - \frac{19\,ic}{720} + \frac{3kc}{164} - \frac{863\,lc}{60480} + \text{\&c. in infinitum.}$$



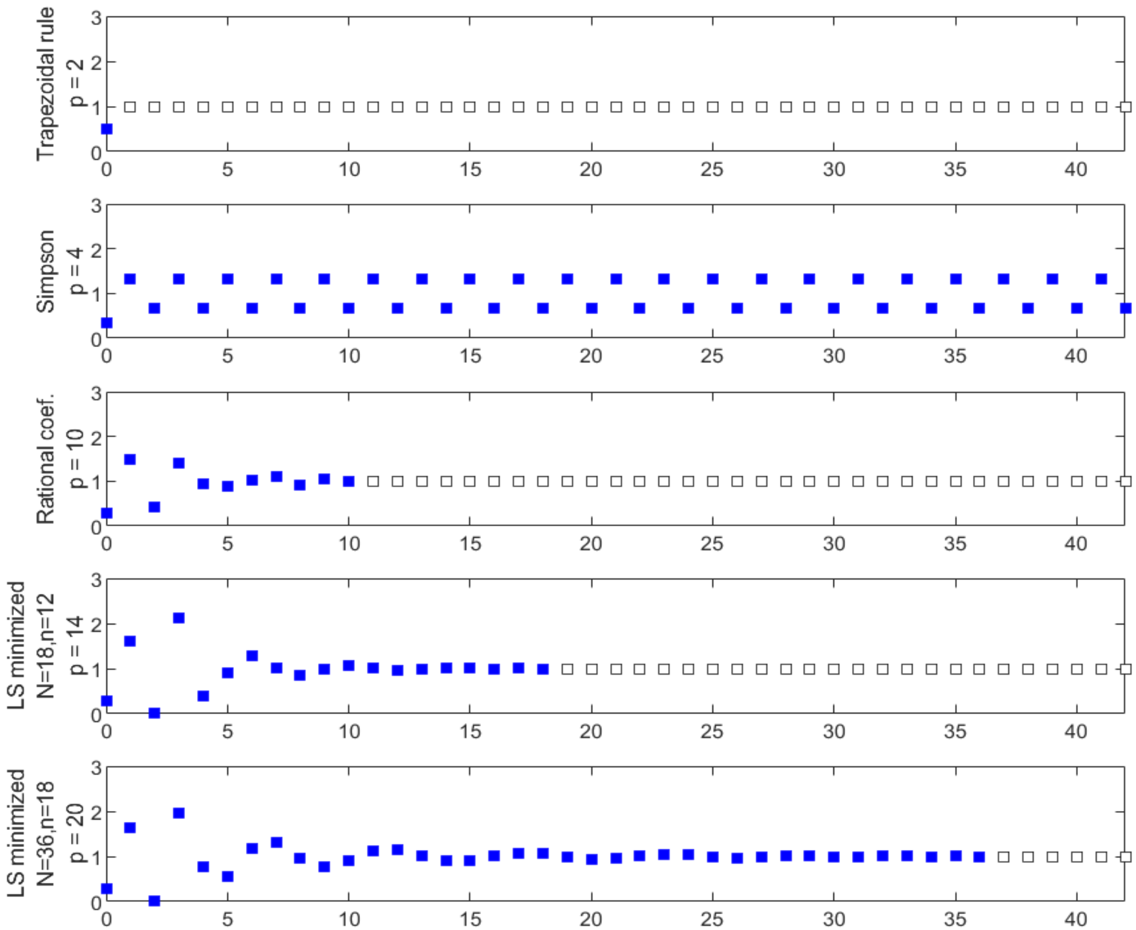
First publications on calculus: Leibniz 1684, Newton 1687.

Comparison of weights, Newton-Cotes' vs. Gregory's methods





Key idea: For a given accuracy order, use somewhat more non-trivial weights than the minimal number in the Gregory formulas



Weight range in Gregory schemes of matching order *p*

[-0.14, 2.24]

[-7.8, 10.2]

[-276, 273]

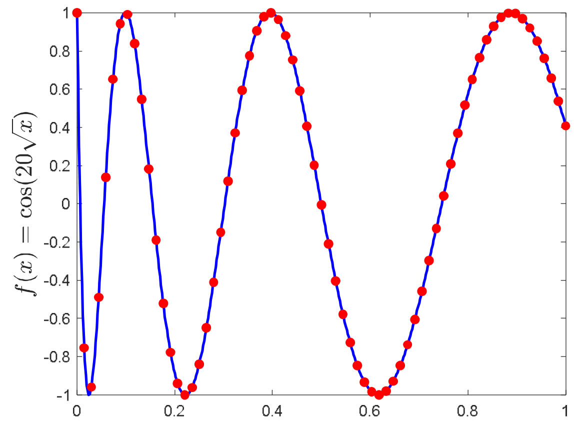
- Corrections from the two sides can overlap.
- Possible to constrict weight sets that are all 'nice' rational numbers (p = 10 case here).

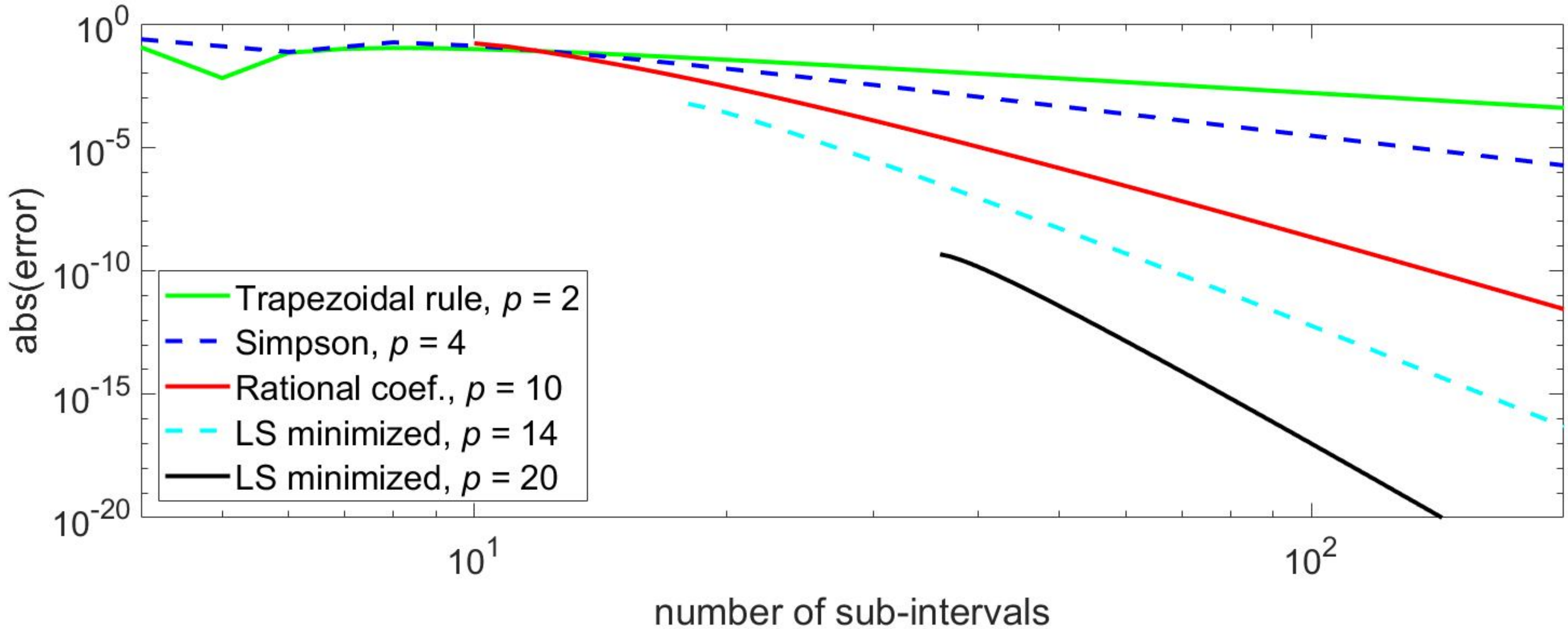
The five quadrature methods applied to a test function

Test function: $f(x) = \cos(20\sqrt{x})$

$$\int_0^1 f(x)dx = \frac{1}{200}\left(\cos(20) + 20\sin(20) - 1\right)$$

Test function with $N = 68$; gives error < 10^{-16}





Some conclusions

Historical notes:

- The pioneering works by Euler, Maclaurin, Plana, Abel, Poisson, etc. were carried out between 200 and 300 years ago.
- Surprisingly little attention has been given in recent years to simplifying and enhancing numerical usage of Euler-Maclaurin-type expansions.

Some aspects of the present numerical approach:

- A variety of finite difference (FD) based end corrections are available for improving the accuracy of the classical TR, requiring no other data than equispaced function values.
- PART 1: Analytic functions given on a grid in the complex plane
- PART 2: Along the real line: Equispaced data surrounding the end point for an infinite sum
- PART 3: Along the real line: Equispaced data only within interval of integration.

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PART 1:

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PART 3:

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(with residue calculus derivations of both the EM and the Abel-Plana formulas)