Some New Perspectives on Finite Differences and the Trapezoidal Rule – Along the Real Axis and in the Complex Plane

Bengt Fornberg

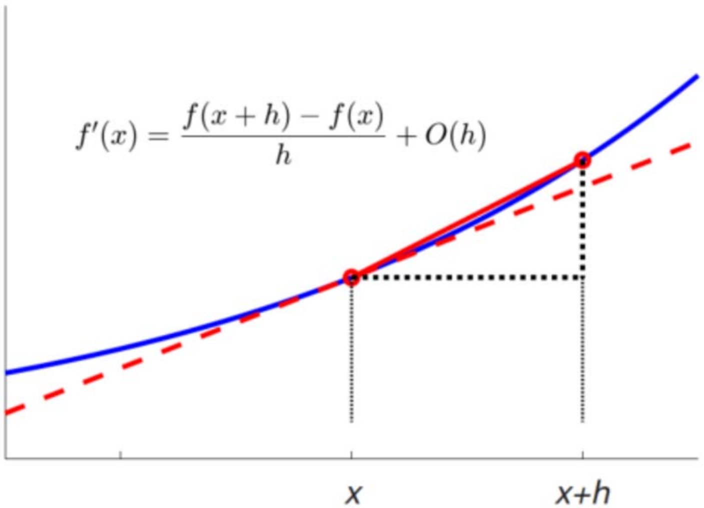
University of Colorado, Boulder
Department of Applied Mathematics

Some FD background

A few historical notes

c 1592 Jost Bürgi (interpolation in trigonometric tables)

17^{th} century Calculus (limit of FD approximations)



19^{th} century ODE solvers in finance and astronomy (e.g., linear multistep methods)

20^{th} century PDE solvers (Richardson, 1911) Led to FEM, FVM, PS methods.

First derivative

order	weights								
2				$-\frac{1}{2}$	0	$\frac{1}{2}$			
4			$\frac{1}{12}$	$-\frac{2}{3}$	0	$\frac{2}{3}$	$-\frac{1}{12}$		
6		$-\frac{1}{60}$	$\frac{3}{20}$	$-\frac{3}{4}$	0	$\frac{3}{4}$	$-\frac{3}{20}$	$\frac{1}{60}$	
8	$\frac{1}{280}$	$-\frac{4}{105}$	$\frac{1}{5}$	$-\frac{4}{5}$	0	$\frac{4}{5}$	$-\frac{1}{5}$	$\frac{4}{105}$	$-\frac{1}{280}$
	↓	↓	↓	↓	↓	↓	↓	↓	↓
PS limit	$\frac{1}{4}$	$-\frac{1}{3}$	$\frac{1}{2}$	-1	0	1	$-\frac{1}{2}$	$\frac{1}{3}$	$-\frac{1}{4}$

Second derivative

order	weights								
2				1	-2	1			
4			$-\frac{1}{12}$	$\frac{4}{3}$	$-\frac{5}{2}$	$\frac{4}{3}$	$-\frac{1}{12}$		
6		$\frac{1}{90}$	$-\frac{3}{20}$	$\frac{3}{2}$	$-\frac{49}{18}$	$\frac{3}{2}$	$-\frac{3}{20}$	$\frac{1}{90}$	
8	$-\frac{1}{560}$	$\frac{8}{315}$	$-\frac{1}{5}$	$\frac{8}{5}$	$-\frac{205}{72}$	$\frac{8}{5}$	$-\frac{1}{5}$	$\frac{8}{315}$	$-\frac{1}{560}$
	↓	↓	↓	↓	↓	↓	↓	↓	↓
PS limit	$-\frac{2}{4^2}$	$\frac{2}{3^3}$	$-\frac{2}{2^2}$	$\frac{2}{1^2}$	$-\frac{\pi^2}{3}$	$\frac{2}{1^2}$	$-\frac{2}{2^2}$	$\frac{2}{3^3}$	$-\frac{2}{4^2}$

Complex plane FD formulas

Analytic functions form a very important special case of general 2-D functions $f(x,y)$.

Definition: With $z = x + iy$ complex, $f(z)$ is *analytic* if

$$\frac{df}{dz} = \lim_{\Delta z \to 0} \frac{f(z+\Delta z) - f(z)}{\Delta z}$$

is uniquely defined, no matter from which direction Δz approaches zero.

Cauchy-Riemann's equations:

Separating $f(z)$ in real and imaginary parts $f(z) = u(x,y) + i\,v(x,y)$,

it holds that $\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \quad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}.$

Some consequences:

FD formulas in the complex x,y-plane, applied to analytic functions, are vastly more efficient / accurate than classical FD formulas.

- No distinction between $\frac{\partial f}{\partial x}$ and $\frac{\partial f}{\partial y}$;
- Cauchy's integral formula: $f^{(k)}(z_0) = \frac{k!}{2\pi i} \oint_\Gamma \frac{f(z)}{(z-z_0)^{k+1}} dz \,, k = 0,1,2,\ldots$

A few examples of complex plane FD formulas

$$f'(0)=\frac{1}{40h}\begin{bmatrix}-1-i & -8i & 1-i\\ -8 & 0 & 8\\ -1+i & 8i & 1+i\end{bmatrix} f+O(h^8),$$

$$f^{(2)}(0)=\frac{1}{20h^2}\begin{bmatrix}i & -8 & -i\\ 8 & 0 & 8\\ -i & -8 & i\end{bmatrix} f+O(h^8),$$

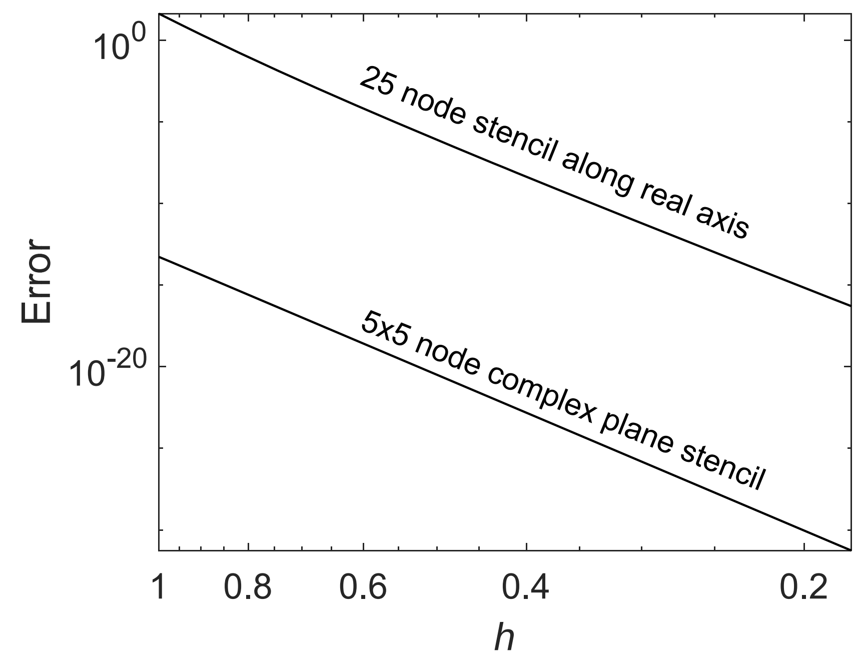
......

$$f^{(4)}(0)=\frac{3}{10h^4}\begin{bmatrix}-1 & 16 & -1\\ 16 & -60 & 16\\ -1 & 16 & -1\end{bmatrix} f+O(h^8),$$

......

$$f^{(8)}(0)=\frac{504}{h^8}\begin{bmatrix}1 & 4 & 1\\ 4 & -20 & 4\\ 1 & 4 & 1\end{bmatrix} f+O(h^4),$$

$$f'(0)=\frac{1}{h}\begin{bmatrix}\frac{1+i}{477360} & \frac{4(-1-i)}{29835} & \frac{i}{1326} & \frac{4(1-i)}{29835} & \frac{-1+i}{477360}\\ \frac{4(-1-i)}{29835} & \frac{8(-1-i)}{351} & \frac{-8i}{39} & \frac{8(1-i)}{351} & \frac{4(1-i)}{29835}\\ \frac{1}{1326} & -\frac{8}{39} & 0 & \frac{8}{39} & -\frac{1}{1326}\\ \frac{4(-1+i)}{29835} & \frac{8(-1+i)}{351} & \frac{8i}{39} & \frac{8(1+i)}{351} & \frac{4(1+i)}{29835}\\ \frac{1-i}{477360} & \frac{4(-1+i)}{29835} & \frac{-i}{1326} & \frac{4(1+i)}{29835} & \frac{-1-i}{477360}\end{bmatrix} f+O(h^{24})$$

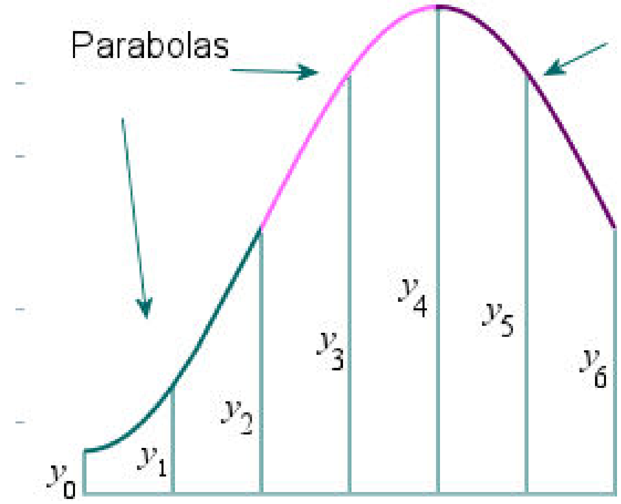


The weights at location μ + iν, with μ,ν integers, decay to zero like $O(e^{-\frac{\pi}{2}(\mu^2+\nu^2)})$

As the accuracy order is increased (or goes to the PS limit), approximations remain highly local.

Extremely high accuracies already for very small stencils. Here approximating $\left.\frac{d^4}{dx^4}e^{2x}\right|_{x=0}$

Simpson and Newton-Cotes formulas



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)

Orders of accuracy increases (from Trap. Rule) 2, 4, 4, 6, 6, 8, 8, …

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.

Gregory's method

With notation

$$\Delta^0 f(x) = f(x)$$
$$\Delta^1 f(x) = f(x+h) - f(x)$$
$$\Delta^2 f(x) = f(x+2h) - 2f(x+h) + f(x)$$
$$\ldots$$

$$\nabla^0 f(x) = f(x)$$
$$\nabla^1 f(x) = f(x) - f(x-h)$$
$$\nabla^2 f(x) = f(x) - 2f(x-h) + f(x-2h)$$
$$\ldots$$

$$\int_{x_0}^{x_N} f(x)dx = h\left[f_0 + f_1 + f_2 + \ldots + f_{N-1} + f_N \right] +$$
$$-\tfrac{1}{2}\left[\Delta^0 f_0 + \nabla^0 f_N\right] + \tfrac{1}{12}\left[\Delta^1 f_0 - \nabla^1 f_N\right] - \tfrac{1}{24}\left[\Delta^2 f_0 - \nabla^2 f_N\right] + \tfrac{19}{720}\left[\Delta^3 f_0 - \nabla^3 f_N\right] - \tfrac{3}{160}\left[\Delta^4 f_0 - \nabla^4 f_N\right] + - \ldots$$

Non-trivial weights at left end; each term increases accuracy order by one.

$p=$	Non-trivial weights								
2	$\frac{1}{2}$								
3	$\frac{5}{12}$	$\frac{13}{12}$							
4	$\frac{3}{8}$	$\frac{7}{6}$	$\frac{23}{24}$						
5	$\frac{251}{720}$	$\frac{299}{240}$	$\frac{211}{240}$	$\frac{739}{720}$					
6	$\frac{95}{288}$	$\frac{317}{240}$	$\frac{23}{30}$	$\frac{739}{720}$	$\frac{157}{160}$				
7	$\frac{19087}{60480}$	$\frac{84199}{60480}$	$\frac{18869}{30240}$	$\frac{37621}{30240}$	$\frac{55031}{60480}$	$\frac{61343}{60480}$			
8	$\frac{5257}{17280}$	$\frac{22081}{15120}$	$\frac{54851}{120960}$	$\frac{103}{70}$	$\frac{89437}{120960}$	$\frac{16367}{15120}$	$\frac{23917}{24192}$		
9	$\frac{1070017}{3628800}$	$\frac{5537111}{3628800}$	$\frac{103613}{403200}$	$\frac{261115}{145152}$	$\frac{298951}{725760}$	$\frac{515677}{403200}$	$\frac{3349879}{3628800}$	$\frac{3662753}{3628800}$	
10	$\frac{25713}{89600}$	$\frac{1153247}{725760}$	$\frac{130583}{3628800}$	$\frac{903527}{403200}$	$-\frac{797}{5670}$	$\frac{6244961}{3628800}$	$\frac{56621}{80640}$	$\frac{3891877}{3628800}$	$\frac{1028617}{1036800}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$ $\ddots$

James Gregory (1638-1675)

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

ponendo $AP = PO = c$

$PB = d$

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

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

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

Transcribed to print by Oxford Univ. Press, 1840

(with them introducing a typo, 164 in place of 160)

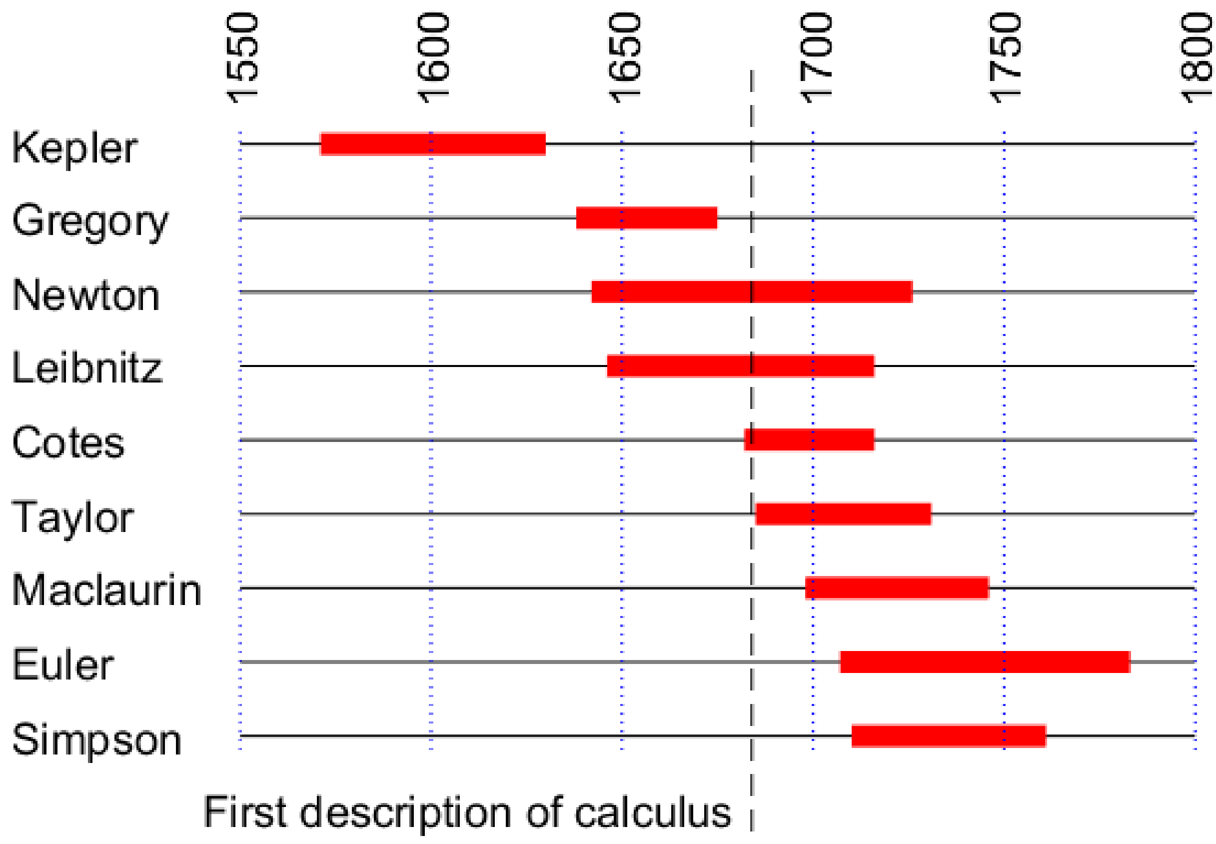
Gregory's exact derivation of this particular expansion is unknown, but he did extensive work on calculus, Taylor expansions, derivatives and integrals in the 1660's. He most likely obtained the coefficients from their *generating function*

$$\frac{1}{\log(1+z)} - \frac{1}{z} = \frac{1}{2} - \frac{1}{12}z + \frac{1}{24}z^2 - \frac{19}{720}z^3 + \frac{3}{160}z^4 - \frac{863}{60480}z^5 + - \ldots$$

Note:

The first publications on calculus:	Gottfried Leibnitz, 1684, Isaac Newton, 1687
Taylor expansions:	Brook Taylor, 1715.

Timeline of the pioneers of numerical quadrature



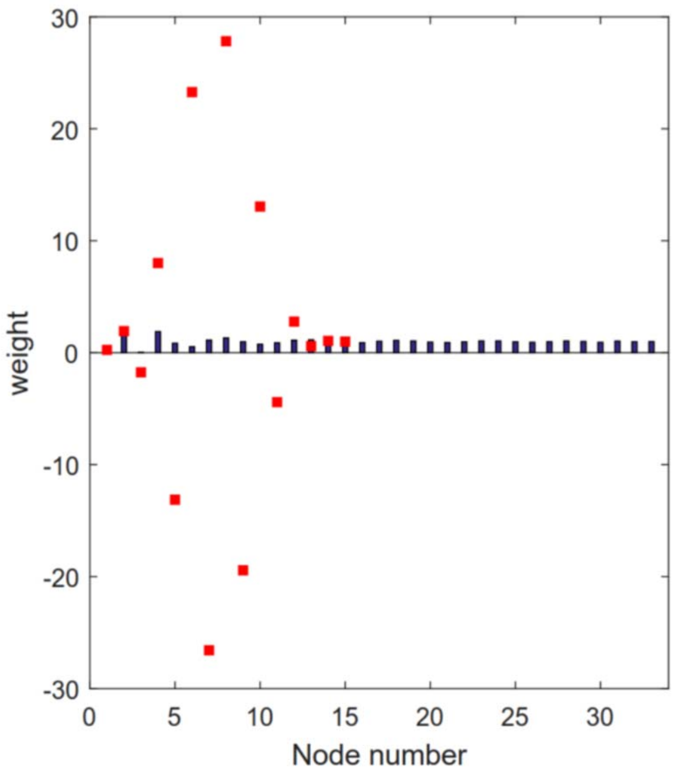
Methods to reach higher orders of accuracy

Gregory:

Modify p weights at each end. Enforcing accuracy $O(h^{p+1})$ leads to p linear relations for p unknowns.

Accuracy enhanced variation:

Modify $N > p$ weights at each end. For accuracy $O(h^{p+1})$, obtain underdetermined linear system. Use the $N - p$ free parameters to ensure all weights positive. In MATLAB, function quadprog. Works up to $p = 20$ (with then $N = 36$)



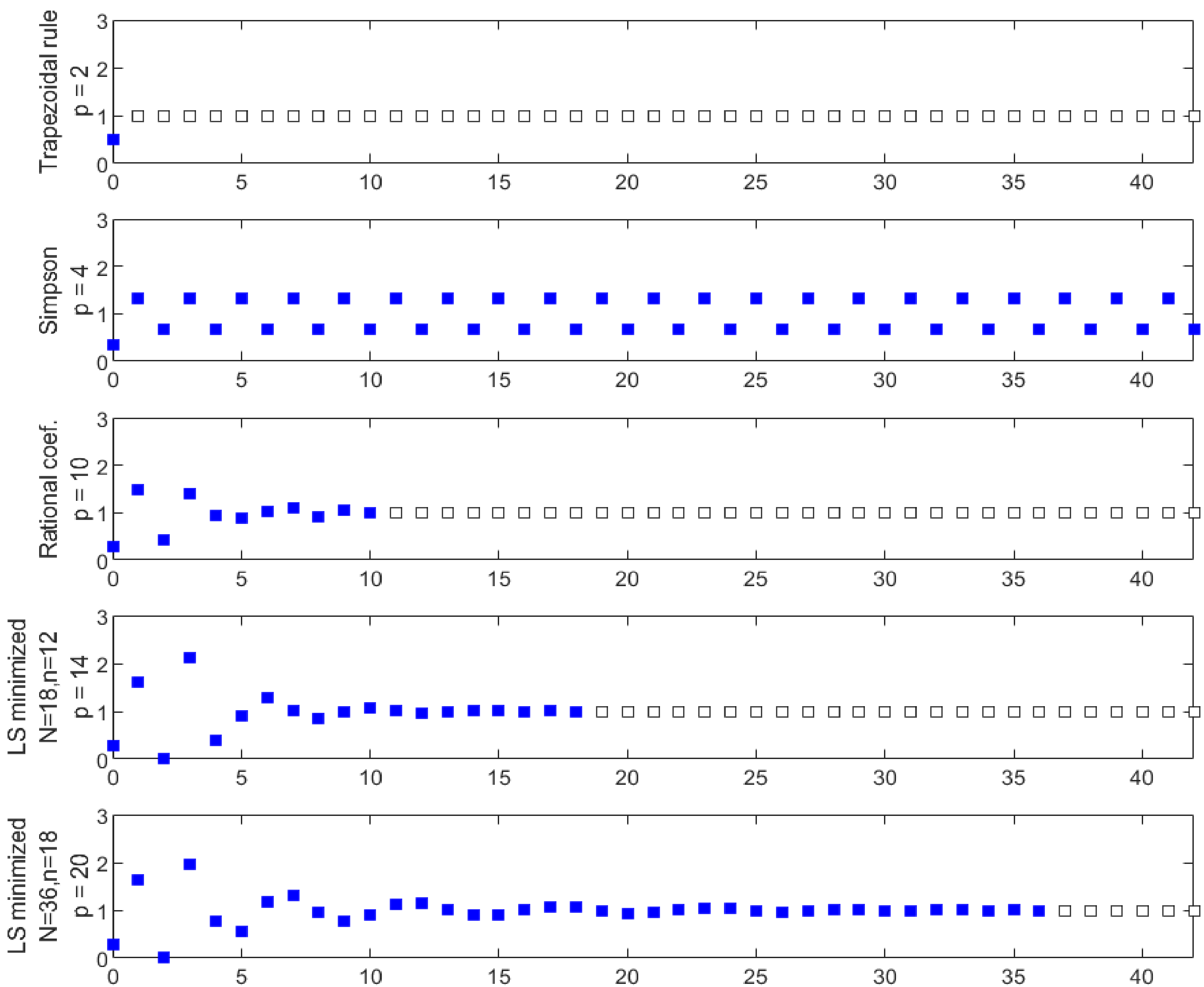
Order $p = 16$ schemes, Gregory vs. L_2-generated

Example of an $O(h^{10})$ scheme with all weights rational and positive

The following set of d_k 'correction' coefficients (weights $w_k = 1 + d_k$) gives an order $p = 10$ scheme:

$$\frac{1}{96}\left\{-\frac{26911}{400}, \frac{628}{1350}, -\frac{10421}{189}, \frac{33487}{840}, -\frac{31441}{4725}, -\frac{16873}{1512}, \frac{10567}{4200}, \frac{10451}{1080}, -\frac{28613}{3024}, \frac{5099}{1400}, -\frac{107}{200}\right\}$$

Illustration of weight sets that will be used in following test



Weight range in Gregory schemes of matching order *p*

[-0.14, 2.24]

[-7.8, 10.2]

[-276, 273]

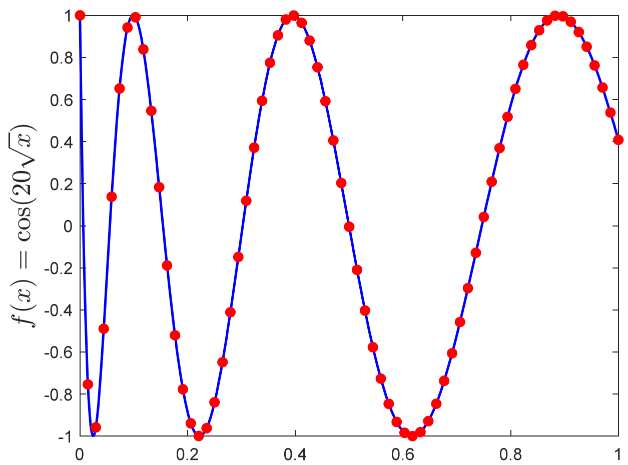
Corrections from the two sides can overlap.
For example rational coefficient scheme can be used on any equispaced node set of 11 or more nodes.

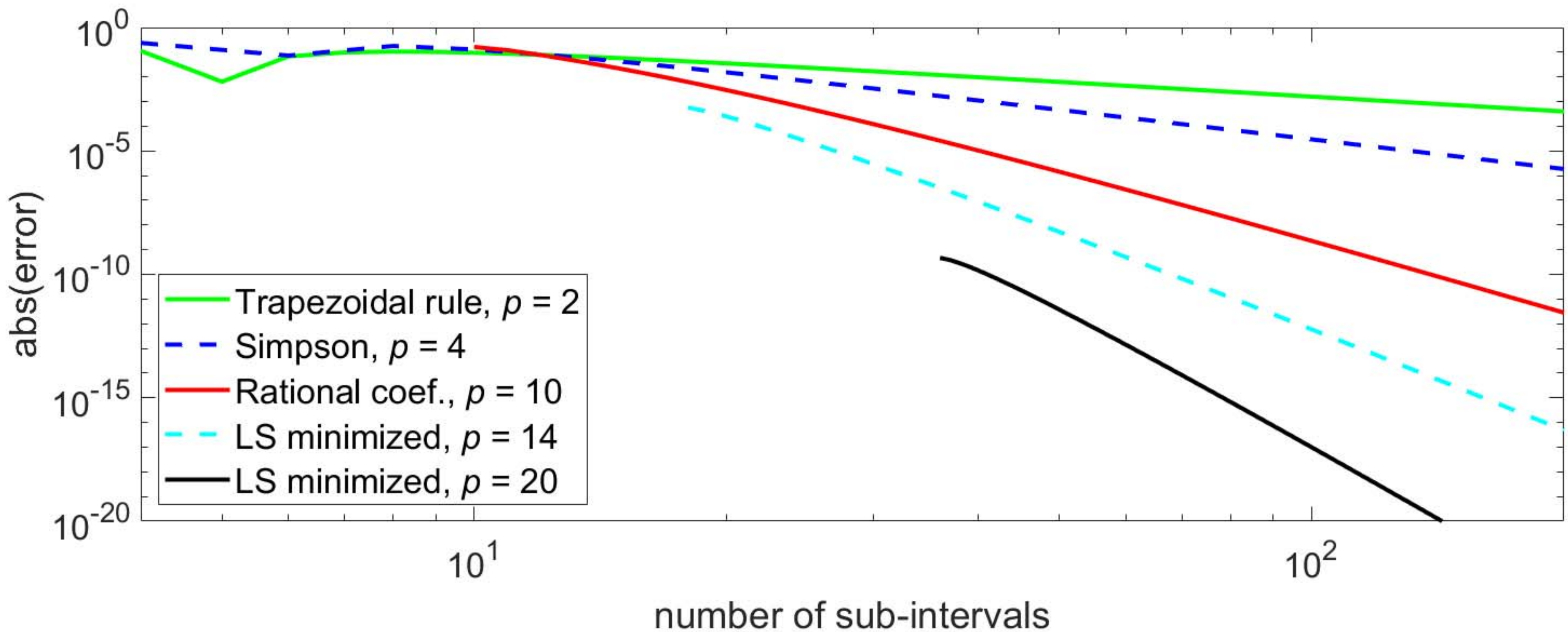
Numerical quadrature methods applied to a test function

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

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

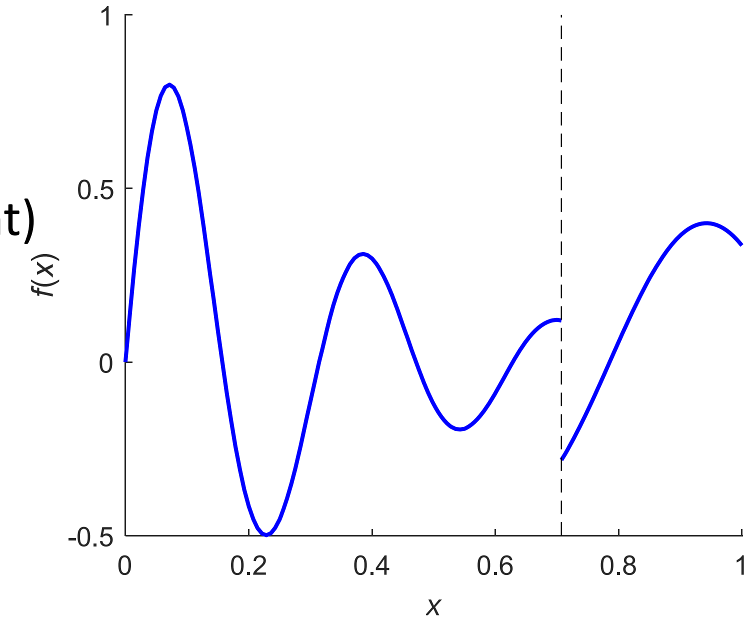
Test function with N = 68; gives error < 10^{-16}





Enhanced TR for discontinuous functions

Work pursued in collaboration with Andrew Lawrence

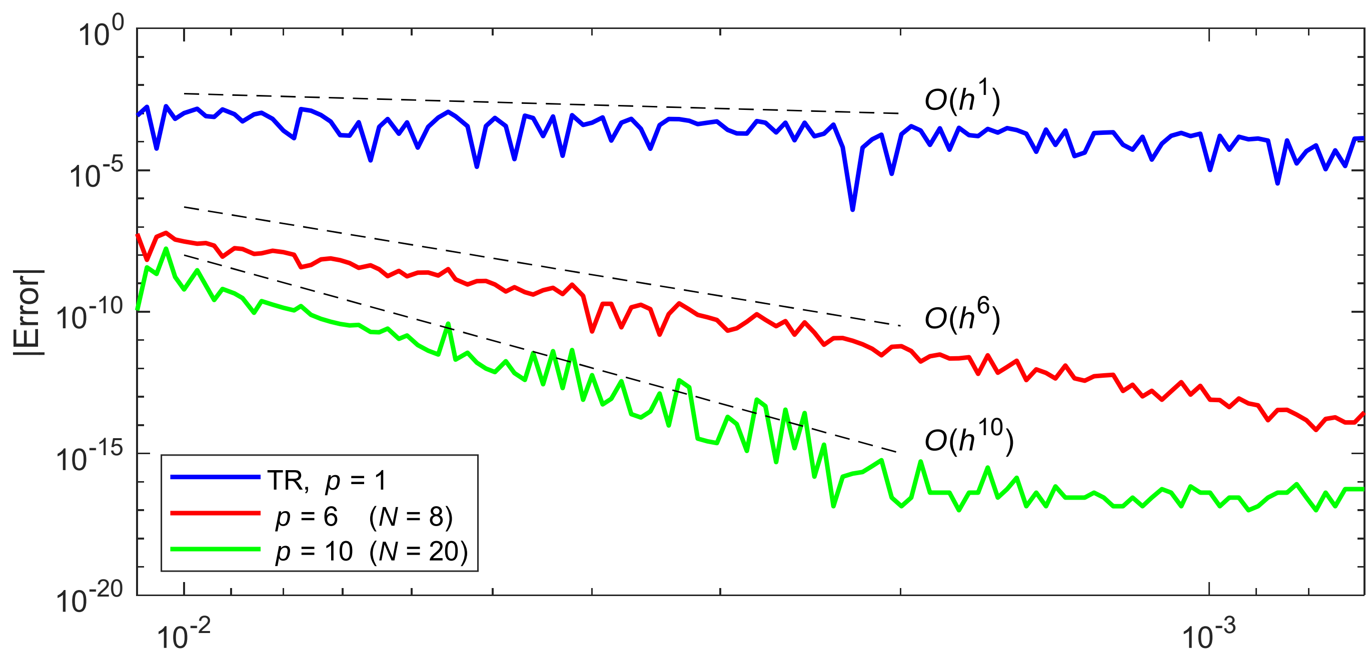


Suppose we know discontinuity location (not at a grid point)

Example:

$$\int_0^1 f(x)\,dx \quad \text{with} \quad f(x) = \begin{cases} e^{-3x}\sin(20x) & , \quad 0 \le x < 1/\sqrt{2} \\ -\dfrac{2}{5}\cos(10x) & , \quad 1/\sqrt{2} \le x \le 1 \end{cases}$$

Apply same idea as above: Use next to discontinuity $N > p$, find positive weights by quadprod. This works up to $p = 10$ in case of using $N = 20$.



Combine FD and enhanced TR: The Euler-Maclaurin formula

$$\int_{x_0}^{\infty} f(x)dx = h\sum_{k=0}^{\infty} f(x_k) - \frac{h}{2} f(x_0) + \frac{h^2}{12} f^{(1)}(x_0) - \frac{h^4}{720} f^{(3)}(x_0) + \frac{h^6}{30240} f^{(5)}(x_0) - \frac{h^8}{1209600} f^{(7)}(x_0) + - \ldots$$

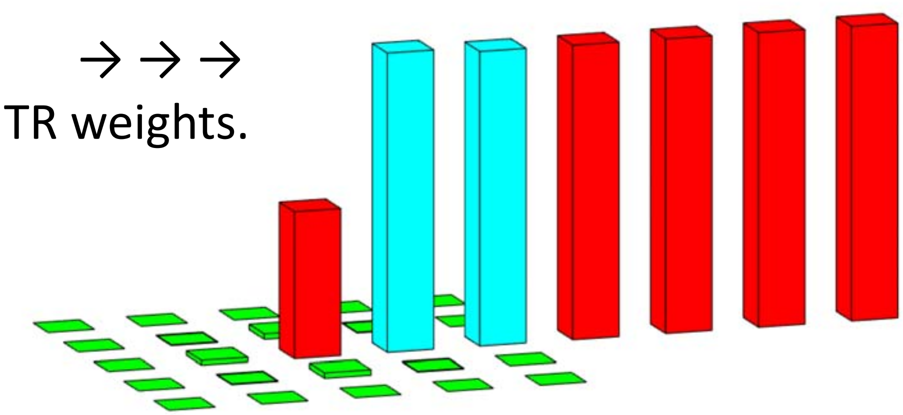
Trapezoidal rule (TR) approximation:

$$\int_0^{\infty} f(x)dx = h\left\{\frac{1}{2} \quad 1 \quad 1 \quad 1 \quad 1 \quad 1 \quad 1 \quad \ldots\right\} f + O(h^2)$$

With 3x3 stencils, one can approximate odd derivatives up through $f^{(7)}(0)$. Doing this gives

$$\int_0^{\infty} f(x)dx = h\left\{\begin{bmatrix} \frac{-821-779i}{403200} & -\frac{1889i}{100800} & \frac{821-779i}{403200} \\ -\frac{1511}{100800} & \left\{\frac{1}{2}\right. & 1+\frac{1511}{100800} \\ \frac{-821+779i}{403200} & \frac{1889i}{100800} & \frac{821+779i}{403200} \end{bmatrix} \left. 1 \quad 1 \quad 1 \quad 1 \quad 1 \quad \ldots \right\}\right\} f + O(h^{10})$$

- Magnitude of weights in 5x5 stencil case →→→
  Correction weights very small compared to TR weights.



- Accuracy order one above the number of stencil points (in figure $O(h^{26})$)

- For finite interval, matching expansion at the opposite end

Easier method to calculate the correction stencil weights

In the case of correcting the trapezoidal rule at the left end $z = 0$:

Consider $\int_0^\infty f(z)dz - \left(\frac{1}{2} f(0) + \sum_{k=1}^{\infty} f(k)\right)$ and apply to $f(z) = e^{z\xi}$. This gives

$$\int_0^\infty e^{z\xi} dz - \left(\frac{1}{2} + \sum_{k=1}^{\infty} e^{k\xi}\right) = \frac{1}{2}\coth\frac{\xi}{2} - \frac{1}{\xi} = -\sum_{k=1}^{\infty} \frac{\zeta(-k)}{k!}\xi^k \qquad (1)$$

Consider a correction stencil with weights w_k at N given nodes z_k, also applied to $f(z) = e^{z\xi}$

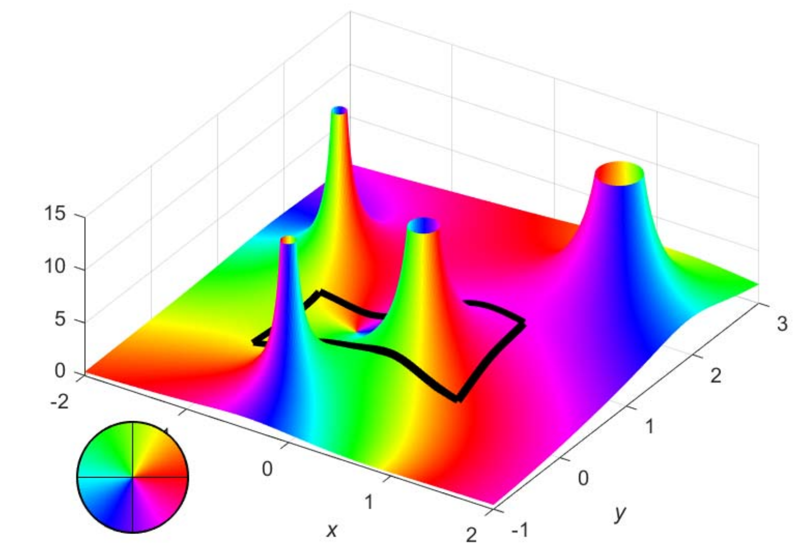
$$\sum_{k=1}^{N} w_k e^{z_k \xi} = \{\text{Taylor expansion in } \xi\} \qquad (2)$$

Equate coefficients for the leading N terms in the expansions (1), (2).
This gives a linear system with a Vandermonde coefficient matrix for the weights w_k.

The order of accuracy of the resulting quadrature approach will match the number of equated coefficients.

For this method, we don't even need to know that the Euler-Maclaurin formula exists (method will be utilized again for fractional derivative generlizations)

Numerically approximate contour integrals in the complex plane



Magnitude and phase angle

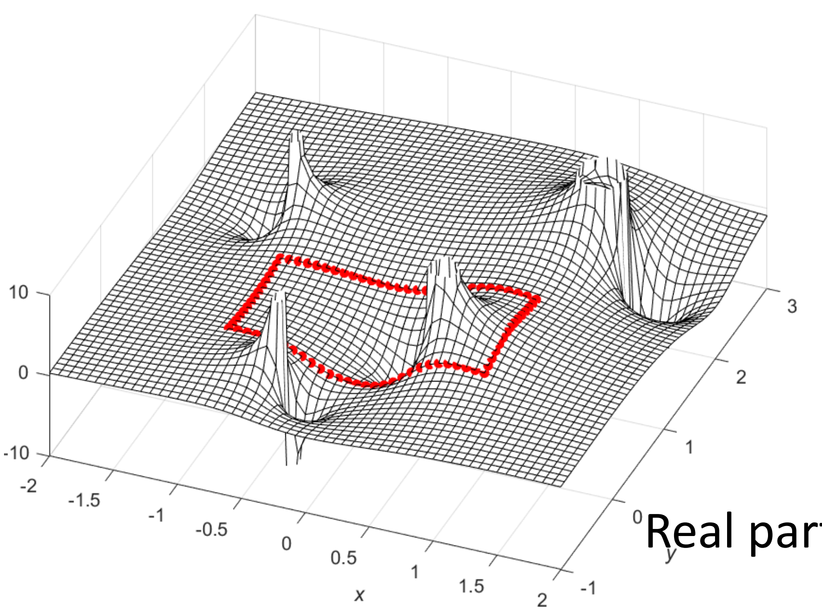
Test function illustrated:

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

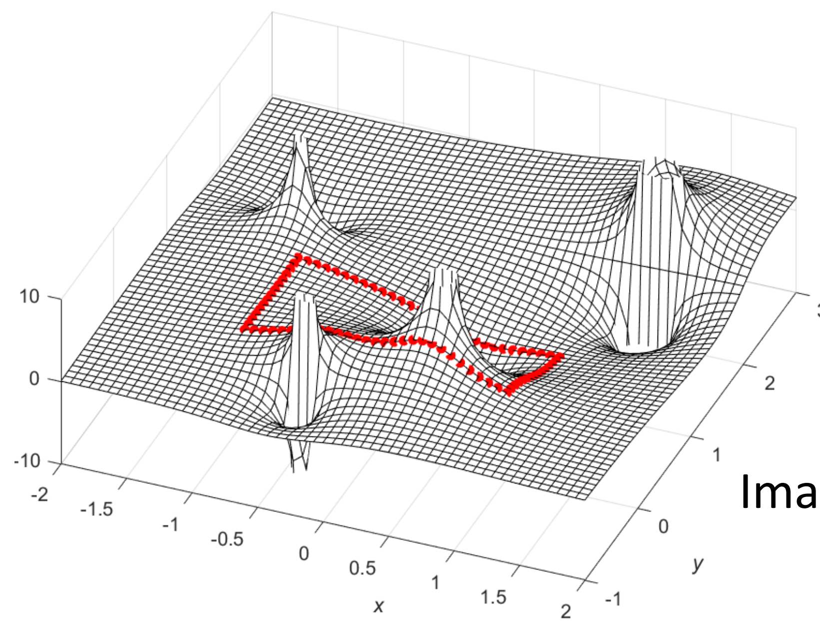
Contours can be open or closed

We want to only use grid point values
(no other functional information)

Using 7x7 'correction stencils' at each path corner gives accuracy ordrer $O(h^{50})$.
Grid density shown sufficient for error around 10^{-40}



Real part

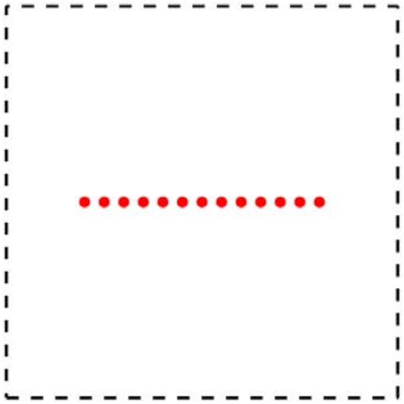


Imaginary part

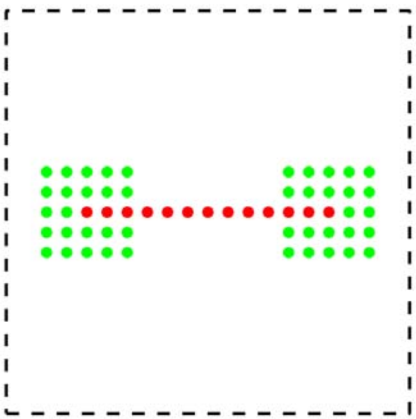
Two main opportunities to improve the trapezoidal rule (TR):

Trapezoidal rule for finite interval

Standard version



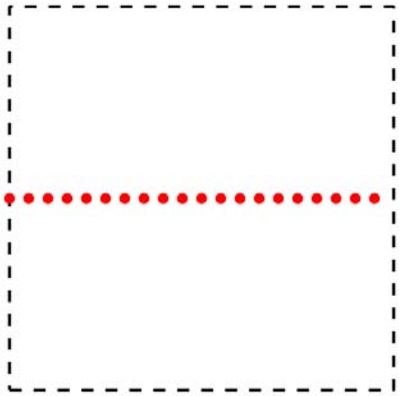
Can one do better?



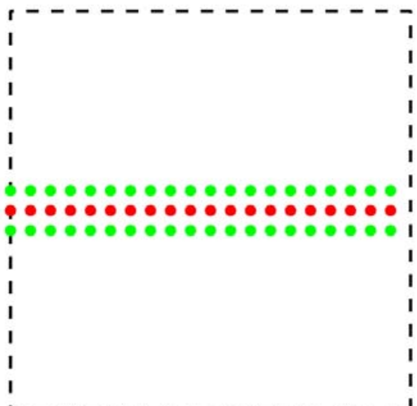
Order of accuracy one more than number of end correction entries

Trapezoidal rule for periodic problem

Standard version

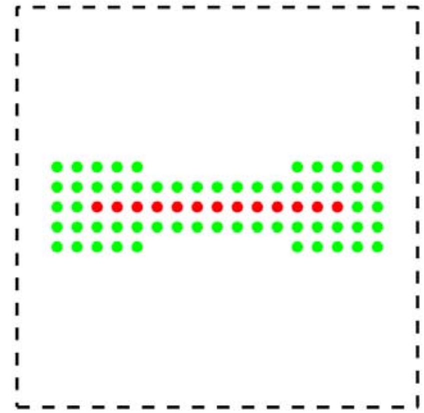


Can one do better?

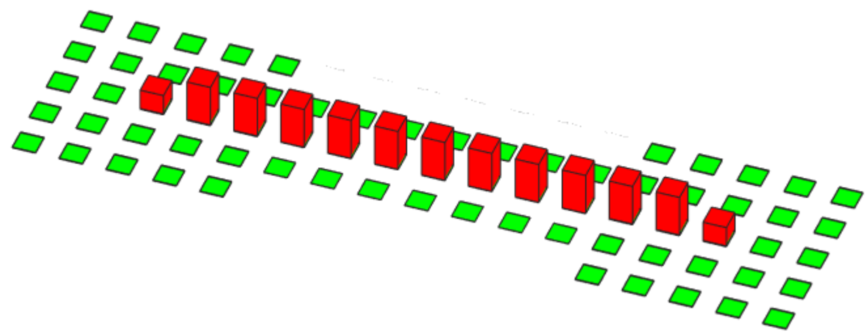


Each pair of lines adds as many correct digits as present in regular TR

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



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



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

Periodic example :

3-line case; weigh together TR sums on adjacent lines by

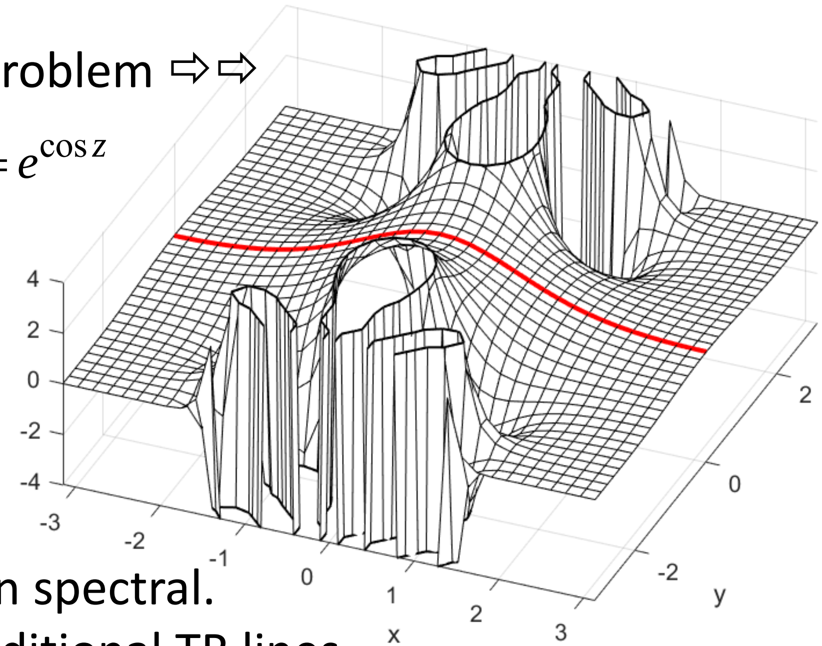
$$\begin{bmatrix} -1/(2\sinh\pi)^2 \\ (1+(\coth\pi)^2)/2 \\ -1/(2\sinh\pi)^2 \end{bmatrix} \approx \begin{bmatrix} -0.001874 \\ 1.003749 \\ -0.001874 \end{bmatrix}$$

5-line case

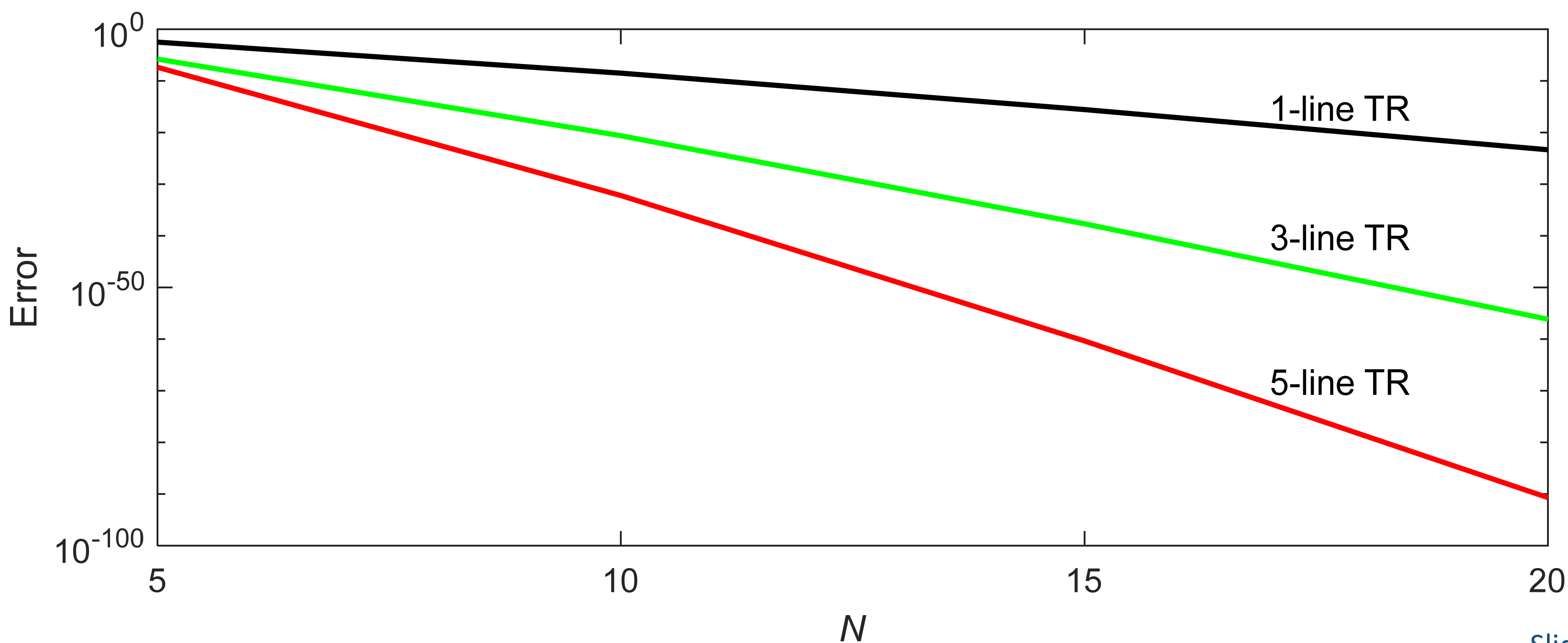
$$\begin{bmatrix} 6.5\cdot 10^{-9} \\ -0.001878 \\ 1.003756 \\ -0.001878 \\ 6.5\cdot 10^{-9} \end{bmatrix}$$

Test problem ⇨⇨

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



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

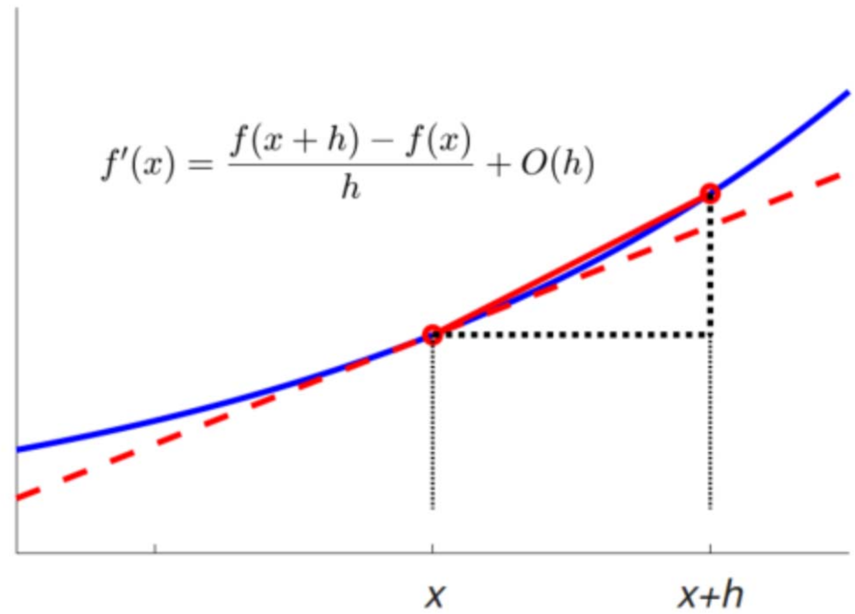


Regular derivatives:

Origin of Calculus

Gregory (1670)
Leibniz (1684), Newton (1687)

First derivative



Fractional derivatives:

Origin of Fractional derivatives

1695 l'Hôpital asked Leibnitz about derivatives of order ½ to which Leibniz replied "This is an apparent paradox from which one day, useful consequences will be drawn"

1823 Abel presented a complete framework for fractional calculus, and a first application

From 1832 Major further contributions by Liouville, Riemann, etc.

Some different ways to introduce fractional derivatives

Fractional integral :

Let $(J\,f)(x) = \int_0^x f(t)dt$ Cauchy: $(J^n f)(x) = \frac{1}{(n-1)!}\int_0^x (x-t)^{n-1} f(f)dt$

Derivatives of x^m :

Let $f(x) = x^m$, then $f^{(n)}(x) = m \cdot (m-1) \cdot \ldots \cdot (m-n+1)\, x^{m-n} = \frac{m!}{(m-n)!} x^{m-n} = \frac{\Gamma(m+1)}{\Gamma(m-n+1)} x^{m-n}$

Fourier series :

Let *f*(*x*) be a real-valued 2π – periodic function. Then

$f(x) = \sum_{\nu=-\infty}^{\infty} c_\nu e^{i\nu x}$ with $c_\nu = \overline{c_{-\nu}}$.

$f^{(n)}(x) = \sum_{\nu=-\infty}^{\infty} c_\nu (i\nu)^n e^{i\nu x}$ One can now make n a fractional number. For example, with $n = 1/2$

$$f^{(1/2)}(x) = \sum_{\nu=-\infty}^{\infty} c_\nu (i\nu)^{1/2} e^{i\nu x} \quad \text{with } (i\nu)^{1/2} = \begin{cases} \frac{1+i}{\sqrt{2}}\sqrt{|\nu|} & ,\nu > 0 \\ \frac{1-i}{\sqrt{2}}\sqrt{|\nu|} & ,\nu < 0 \end{cases} \Rightarrow f^{(1/2)}(x) \text{ also real-valued.}$$

Fractional derivatives are not unique:

It was recently (2022) discovered that all main versions belong to a two-parameter family.

Two most commonly used types of fractional derivatives

Riemann-Liouville (1832, 1847):

$$ {}_{0}^{RL}D_t^{\alpha} f(t) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dt^n} \int_0^t \frac{f(\tau)}{(t-\tau)^{\alpha+1-n}} d\tau, \qquad n-1 < \alpha < n $$

- For m integer $D^{\alpha+m} f(t) = D^m D^{\alpha} f(t)$
- Limit $\alpha \to$ integer is continuous

Caputo (1967):

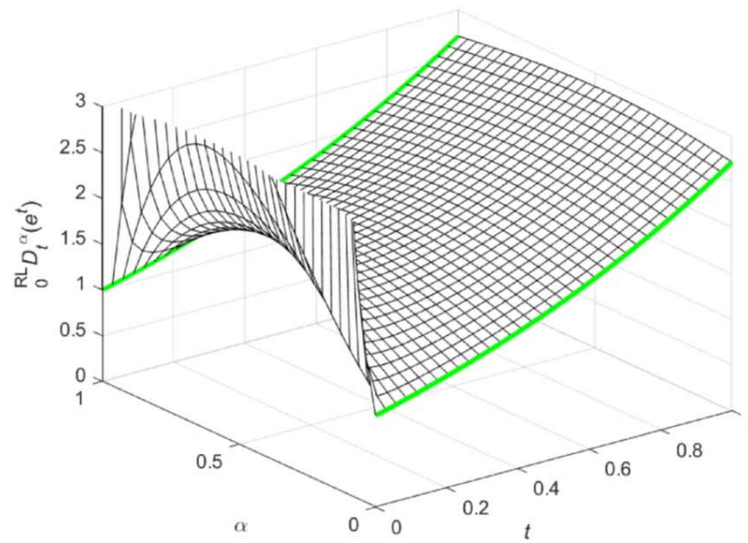
$$ {}_{0}^{C}D_t^{\alpha} f(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t \frac{\frac{d^n}{d\tau^n} f(\tau)}{(t-\tau)^{\alpha+1-n}} d\tau, \qquad n-1 < \alpha < n $$

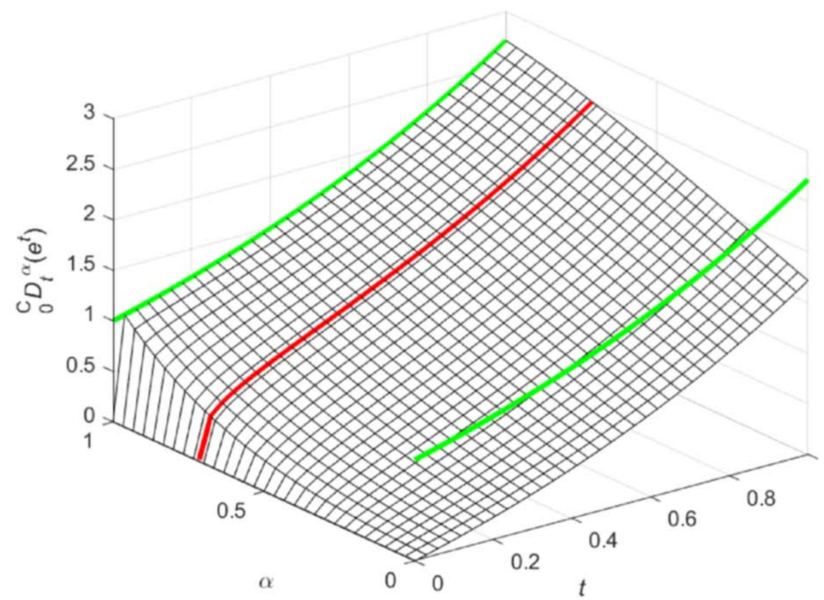
- For m integer $D^{\alpha+m} f(t) = D^{\alpha} D^m f(t)$
- D(constant) = 0
- Solving fractional ODEs requires easy initial conditions ICs

Note also:

- Singularity at $t = 0$ (branch point if t complex)
- $$ {}_{0}^{RL}D_t^{\alpha} f(t) = {}_{0}^{C}D_t^{\alpha} f(t) + \sum_{k=0}^{n-1} \frac{t^{k-\alpha}}{\Gamma(k+1-\alpha)} f^{(k)}(0). $$

Fractional erivatives of e^t





What are fractional derivatives useful for?

- Fractional diffusion

  Recall heat / diffusion equation $u_t = u_{xx}$.

  i. Fractional in time, $D^{\alpha}{}_{t}\, u = u_{xx}$ with $\alpha \approx 1$, provides 'memory'

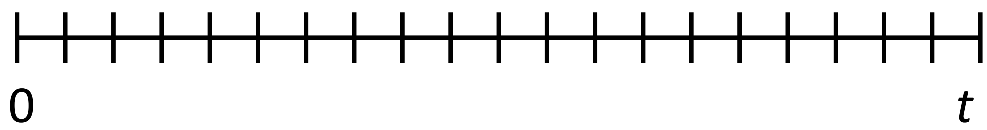
  ii. Fractional in space, $u_t = D^{\alpha}{}_{x}\, u$ with $\alpha \approx 2$, often represents better various 'anomalous' diffusion processes (typically with 'base point' on each side).

- Frequency-dependent wave propagation
- Random walks
- Active damping of flexible structures
- Gas/solute transport/reactions in porous media
- Epidemiology (incl. asymptomatic spreading)
- Modeling of bone/tissue growth/healing
- Modeling of shape memory materials
- Economic processes with memory
- Modeling of supercapacitors / advanced batteries using nano-materials

How to numerically compute fractional derivatives, *t* real

Recall Caputo: $D^{\alpha} f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\frac{d}{d\tau} f(\tau)}{(t-\tau)^{\alpha}} d\tau, \qquad 0 < \alpha < 1$

Equispaced grid in *t*-direction

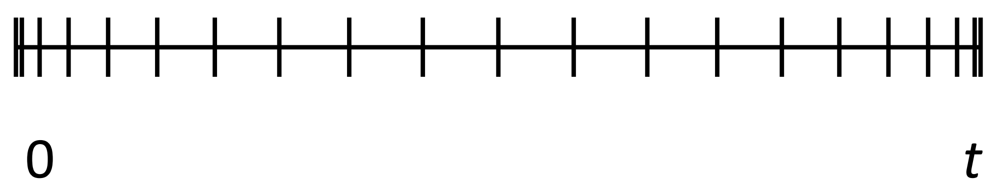


Grünwald-Letnikov formula: (1868)

$$ {}^{RL}D^{\alpha} f(t) = \lim_{h->0} \frac{\Sigma_{GL}}{h^{\alpha}} \quad \text{where} \quad \Sigma_{GL} = \sum_{j=0}^{[t/h]} (-1)^j \binom{\alpha}{j} f(t - jh). $$

Still dominant in computing; only first order accurate – Error $O(h^1)$.
Improvements available up to around $O(h^4)$.

Nodes in *t*-direction at prescribed non-equispaced locations



Spectral methods reminiscent of Gaussian quadrature possible.
This type of node sets are impractical in time for fractional order ODEs / PDEs.

Apply complex plane integration approach to fractional derivative calculations

Work pursued in collaboration with Cécile Piret, Caleb Jacobs, Andrew Lawrence, and Austin Higgins

Recall again Caputo derivative: $$D^{\alpha} f(z) = \frac{1}{\Gamma(1-\alpha)} \int_0^z \frac{f'(\tau)}{(z-\tau)^{\alpha}} d\tau, \qquad 0 < \alpha < 1$$

Theorem: If $f(z)$ is analytic, so is $D^{\alpha} f(z)$ (typically with branch point at $z = 0$).

Preliminary step for numerics: Integrate by parts once, to get $f(\tau)$ instead of $f'(\tau)$.

Key result: One can obtain equally high order accurate TR end correction stencils also for the singular end point $\tau = z$ of the integrand.

An additional technicality is needed when the evaluation point z is close to the base point 0.

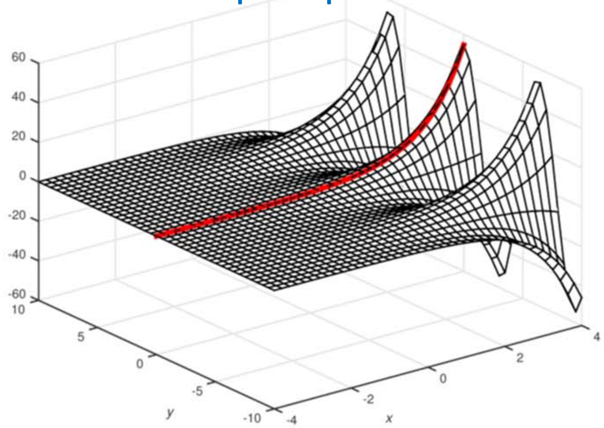
Procedure: Follow grid lines with TR and end correct wit 5x5 stencils at base point, evaluation point, and at any path corner.

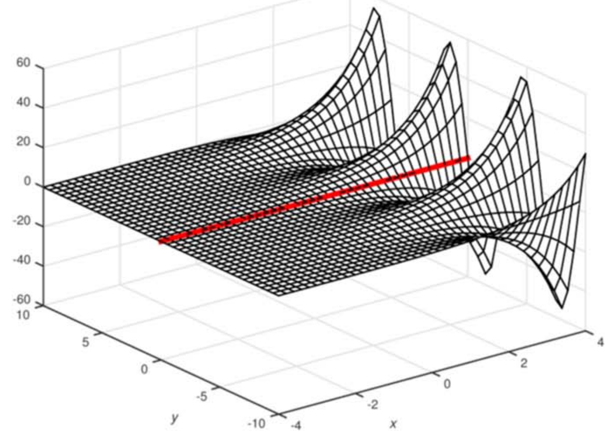
Fractional derivative illustrations:

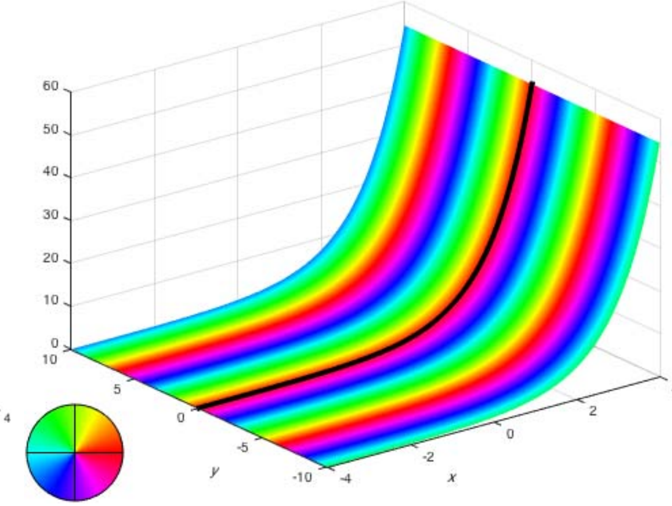
$f(z) = e^{z}$

Displayed grid densities sufficient for machine precision 10^{-16} accuracy

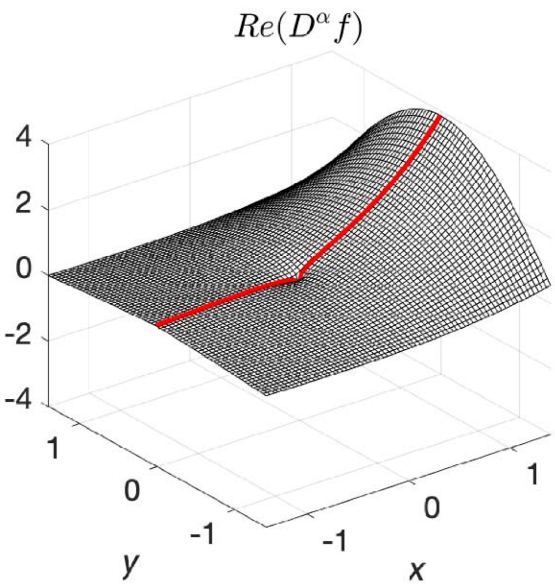
Function in complex plane:

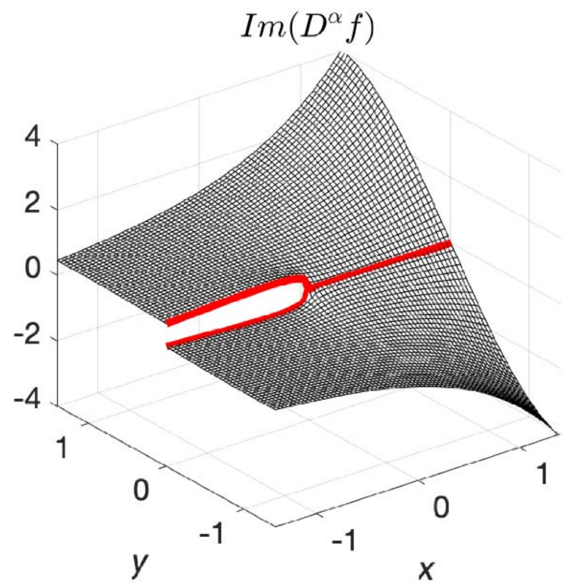


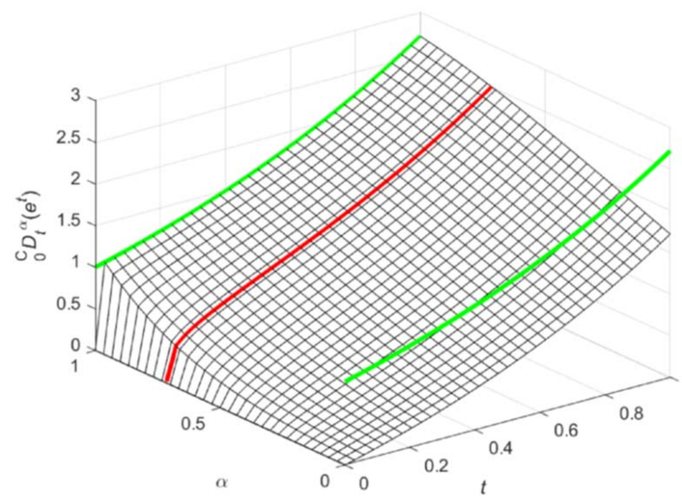




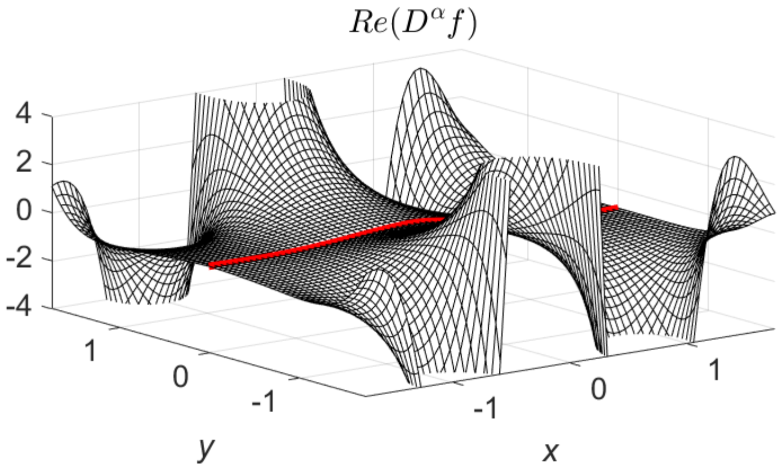
Fractional derivative, shown in the case of α = 5/7

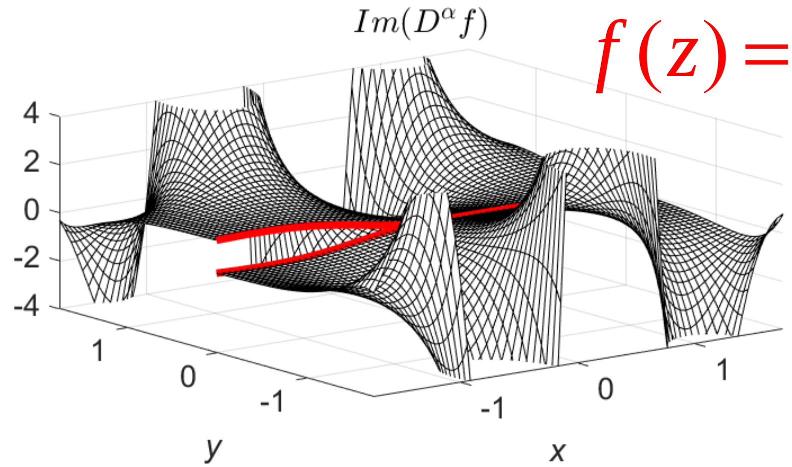






Exact: $$D^{\alpha} e^{z} = e^{z}\left(1 - \frac{\Gamma(1-\alpha, z)}{\Gamma(1-\alpha)}\right)$$

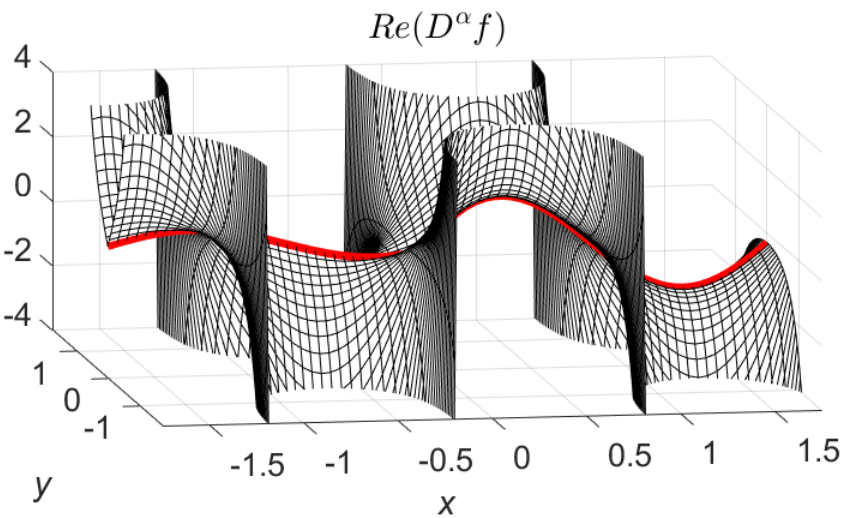


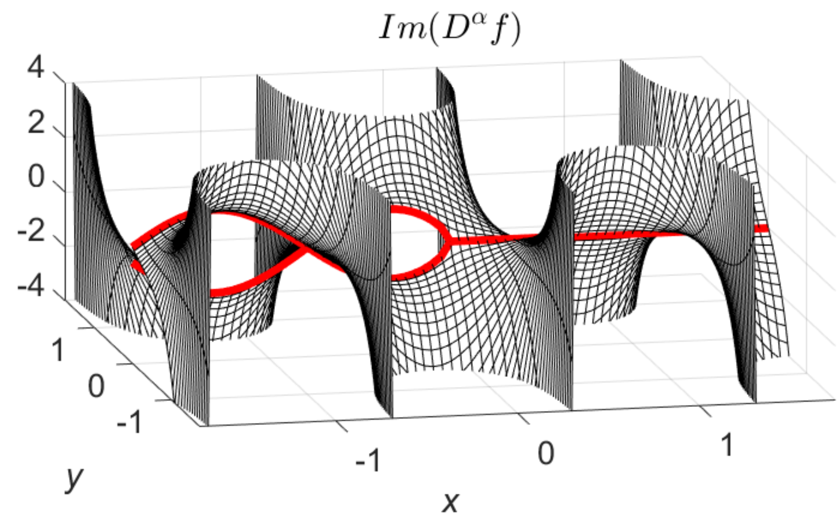


$$f(z) = e^{-z^2}$$

$$D^{1/3}e^{-z^2} = -\frac{9z^{5/3}}{5\Gamma(2/3)}\,{}_2F_2\left(1,\tfrac{3}{2};\tfrac{4}{3},\tfrac{11}{6};-z^2\right)$$

$$f(z) = \sin \pi z$$





$$D^{\pi/8}\sin \pi z = \frac{\pi\, z^{1-\pi/8}}{\Gamma(1-\frac{\pi}{8})}\,{}_1F_2(1;1-\tfrac{\pi}{8},\tfrac{3}{2}-\tfrac{\pi}{16};-\tfrac{\pi^2 z^2}{4})$$

Further fractional derivative research opportunities that are currently pursued:

- Change present complex plane method to be applicable along the real axis.

- Solve fractional order ODEs to high orders of accuracy.

- Evaluations of special functions (especially hypergeometric). For example:

$$
\begin{aligned}
{}_1F_1(a;c;z) &= \frac{\Gamma(c)}{\Gamma(b)} z^{1-c} D_z^{a-c}[e^z z^{a-1}] \\
{}_2F_1(a,b;c;z) &= \frac{\Gamma(c)}{\Gamma(a)} z^{1-c} D_z^{b-c}[z^{b-1}(1-z)^a] \\
{}_{p+1}F_{q+1}(\ldots;\ldots;z) &= \begin{Bmatrix} \text{simple} \\ \text{function} \end{Bmatrix} \times \begin{Bmatrix} \text{fractional} \\ \text{deriv. of} \end{Bmatrix} \left(z^c \, {}_pF_q(\ldots;\ldots;z) \right)
\end{aligned}
$$

Some conclusions

Finite differences (FD)

- Derivatives of grid-based analytic functions can be evaluated to very high levels of accuracy already on coarse grids.

Trapezoidal rule (TR) enhancements:

- Very high levels of accuracy can be reached using only equispaced data within the integration interval. The integrand may be discontinuous at some known location(s).
- With grid data in the complex plane, contour integration of analyticv functions readily reach accuracy orders such as $O(h^{50})$.

Fractional derivatives:

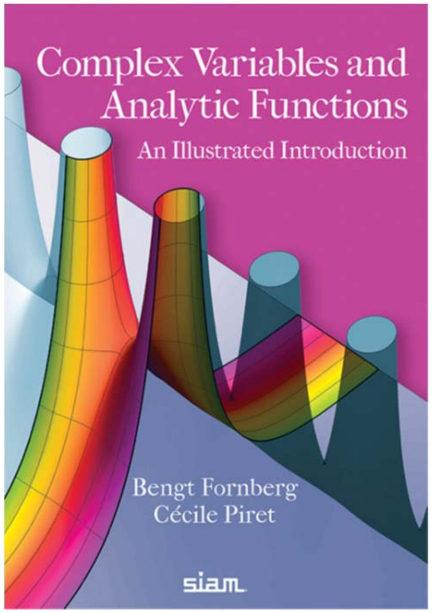
- Fractional derivatives of analytic functions can be computed to machine precision accuracy using grids with density comparable to what is needed for typical functional displays.

New opportunities for 3-D harmonic functions:

- Highly accurate FD approximations available.

Two books relevant to this presentation:

B.F. and C. Piret, ***Complex Variables and Analytic functions: An Illustrated Introduction***, SIAM (2020). → → →



B.F. ***High Accuracy Finite Difference Methods***, Cambridge University Press (to be published in 2024).