Finite Difference Formulas and Numerical Contour Integration in the Complex Plane

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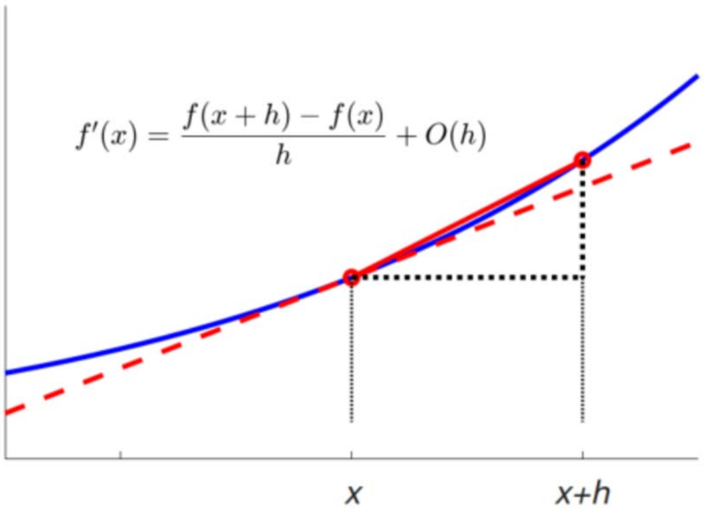
Some FD background

A few historical notes

c 1592 — Jost Bürgi (interpolation in trigonometric tables)

17th century — Calculus (limit of FD approximations)



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

20th 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	$\frac{4}{5}$	$-\frac{1}{5}$	$\frac{4}{105}$	$-\frac{1}{280}$
	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$
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	$-\frac{1}{560}$	$\frac{8}{315}$	$-\frac{1}{5}$	$\frac{8}{5}$	$-\frac{205}{72}$	$\frac{8}{5}$	$-\frac{1}{5}$	$\frac{8}{315}$	$-\frac{1}{560}$
	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$
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

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

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

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

$$f''(0) = \frac{1}{20h^2}\begin{bmatrix} i & -8 & -i \\ 8 & 0 & 8 \\ -i & -8 & i \end{bmatrix} f + O(h^7),$$

......

$$f^{(4)}(0) = \frac{3}{10h^4}\begin{bmatrix} -1 & 16 & -1 \\ 16 & -60 & 16 \\ -1 & 16 & -1 \end{bmatrix} f + O(h^5),$$

......

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

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

For p^{th} derivative, the accuracy is $O(h^{\{\text{number of stencil points}\} - p})$

Extremely high accuracies already for very small stencils

The weights at location μ + iν, 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), apptoximations remain highly local.

Example of application: 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:

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

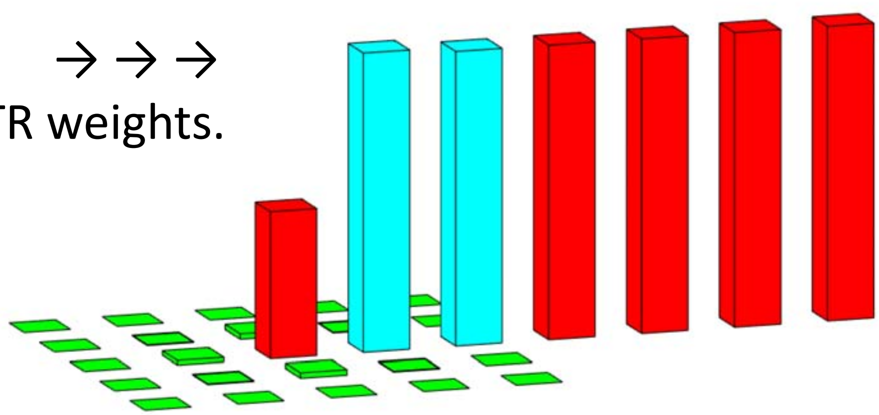
With 3x3 stencils, one can approximate odd derivatives up through $f^{(7)}(0)$. Doing this gives

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

- 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 $O(h^{24})$)

- 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 $f(z) = e^{z\xi}$

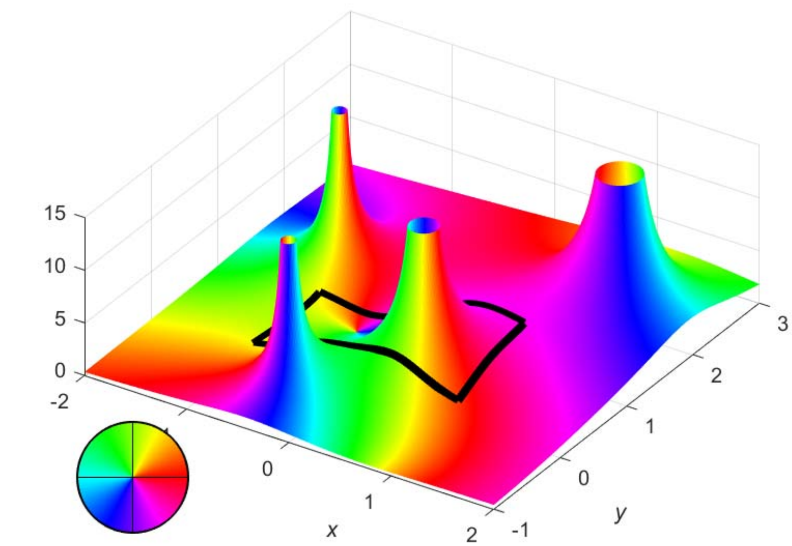
$$\sum_{k=1}^{N} w_k e^{z_k \xi} = \left\{ \text{Taylor expansion in } \xi \right\} \qquad (2)$$

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

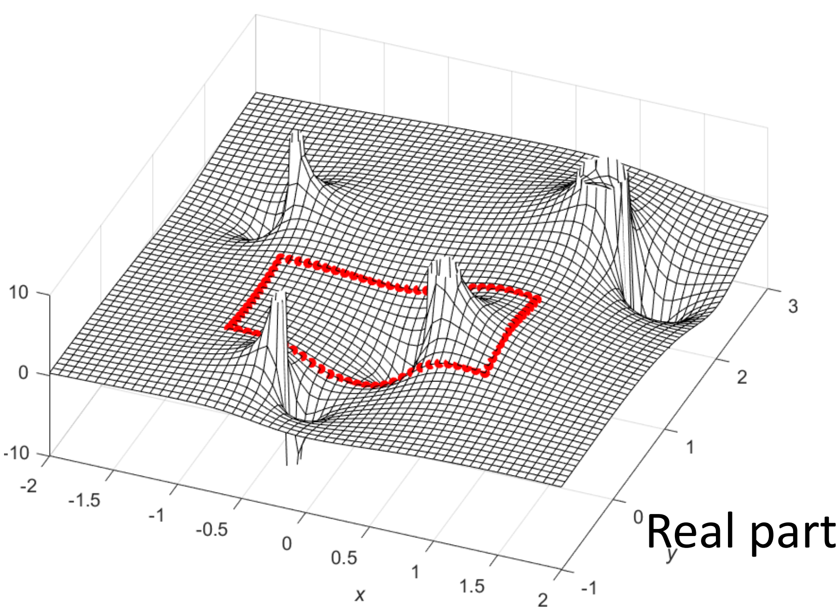
Test function illustrated:

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

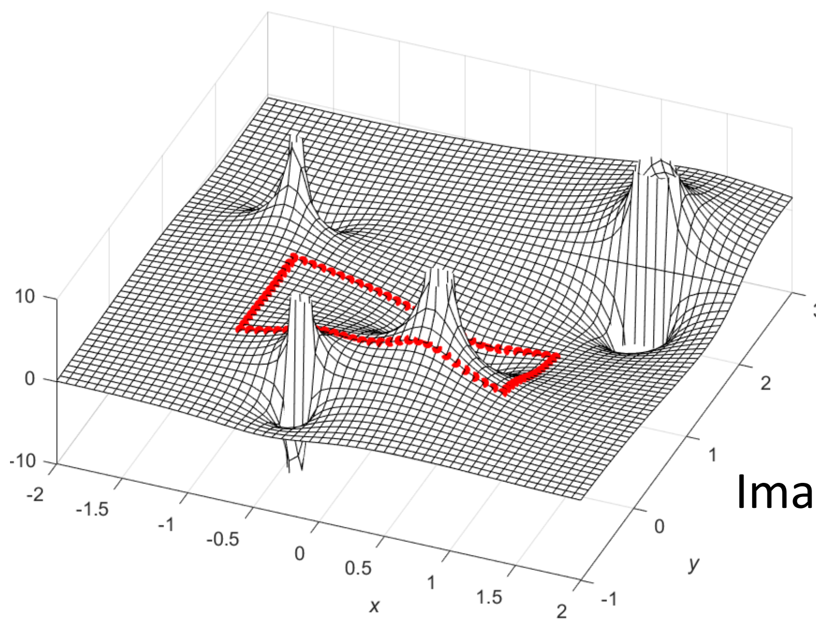
Contours can be open or closed

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

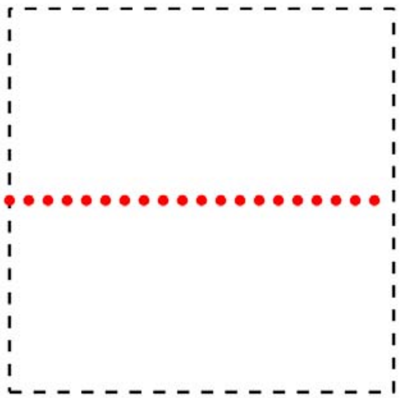


Imaginary part

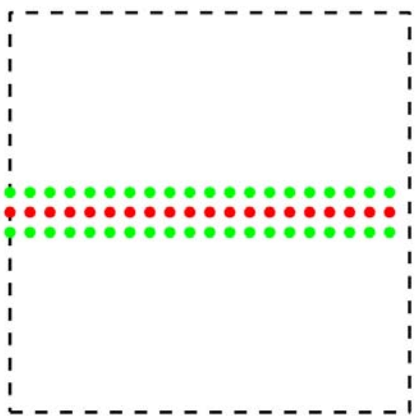
Two main opportunities to improve the trapezoidal rule (TR):

Trapezoidal rule for periodic problem

Standard version



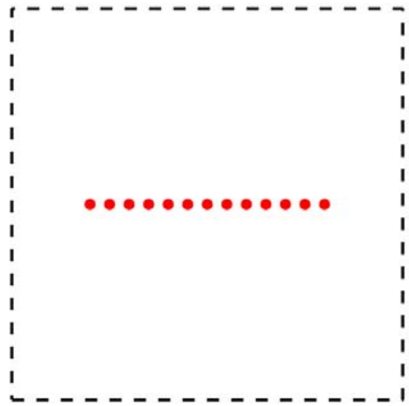
Can one do better?



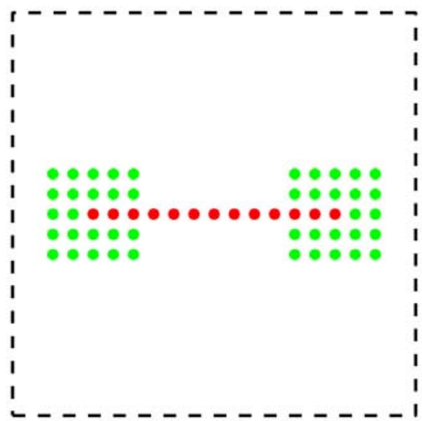
Each pair of lines adds as many correct digits as present in regular TR

Trapezoidal rule for finite interval

Standard version

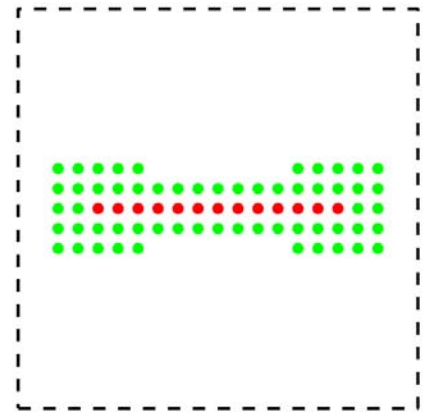


Can one do better?



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)

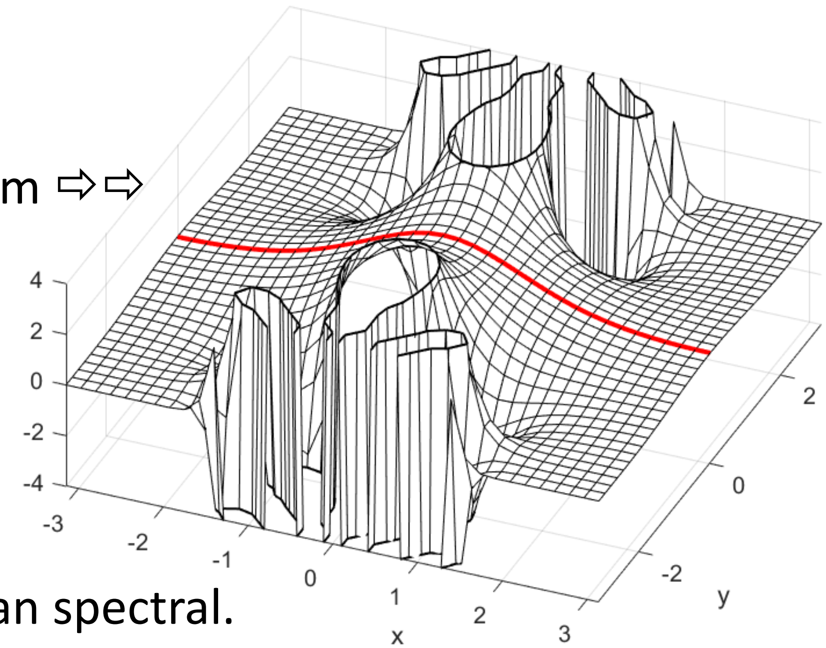
Periodic example :

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

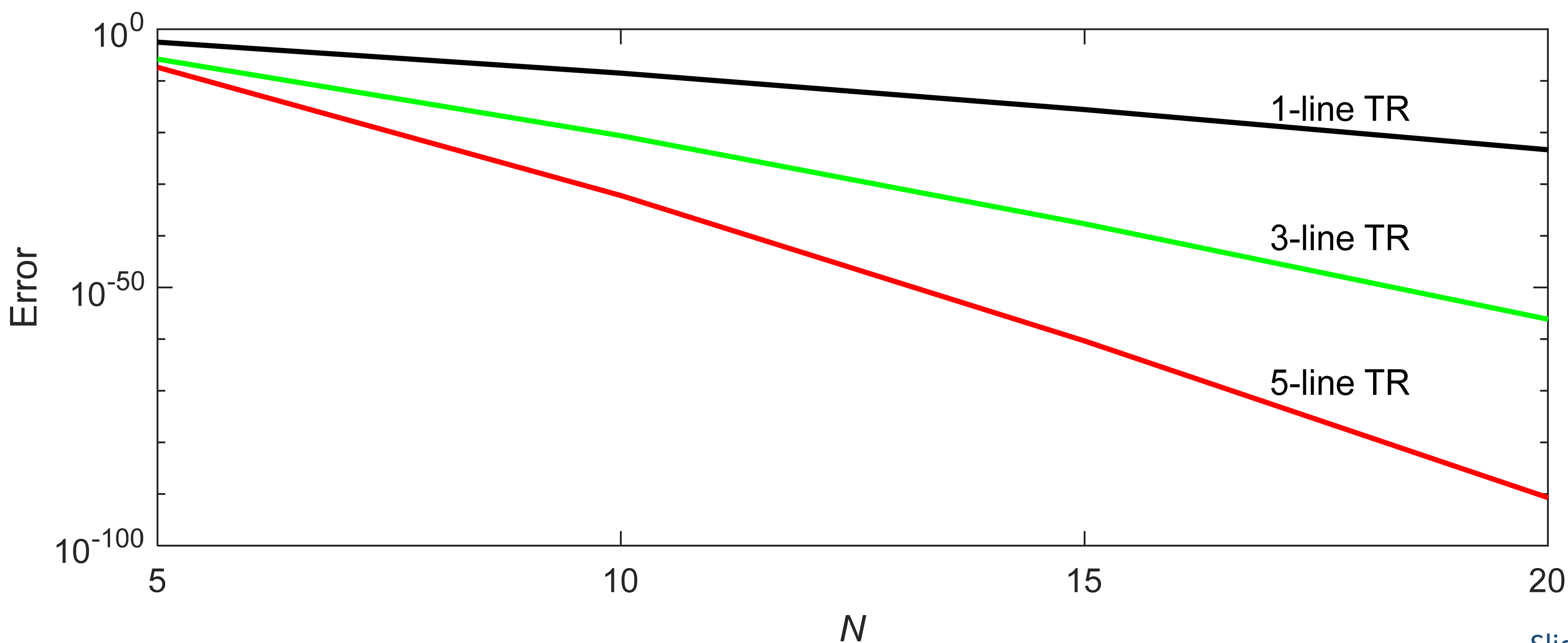
$$\begin{bmatrix} -1/(2\sinh\pi)^2 \\ (1+(\coth\pi)^2)/2 \\ -1/(2\sinh\pi)^2 \end{bmatrix} \approx \begin{bmatrix} -0.00187 \\ 1.00375 \\ -0.00187 \end{bmatrix}$$

Test problem ⇨⇨

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



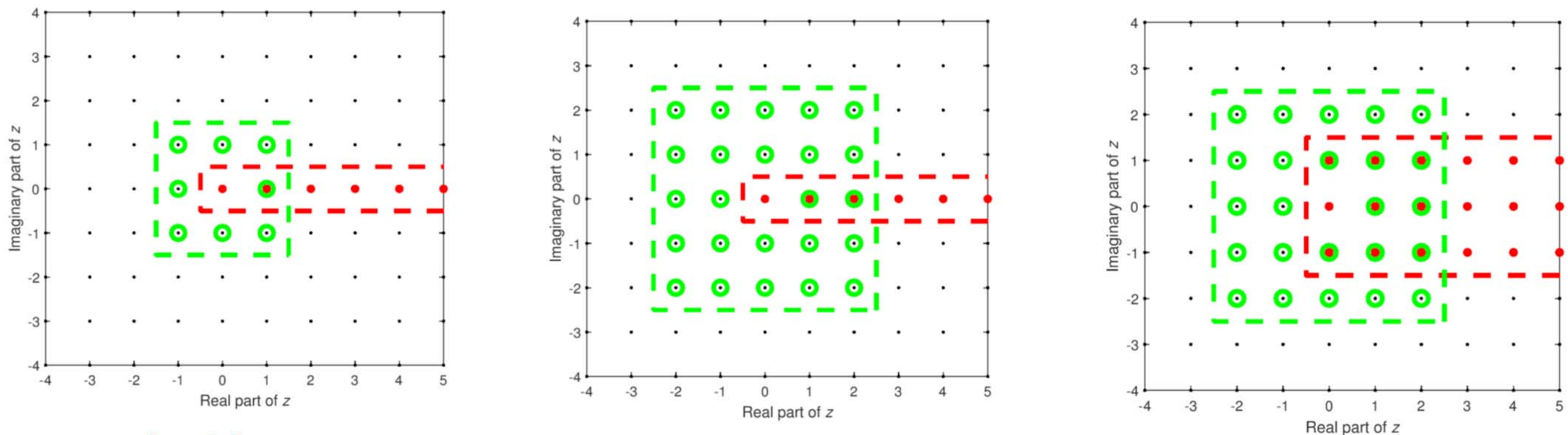
Log-linear plot below – convergence slightly better than spectral.
Number of correct digits increases as expected with additional TR lines.



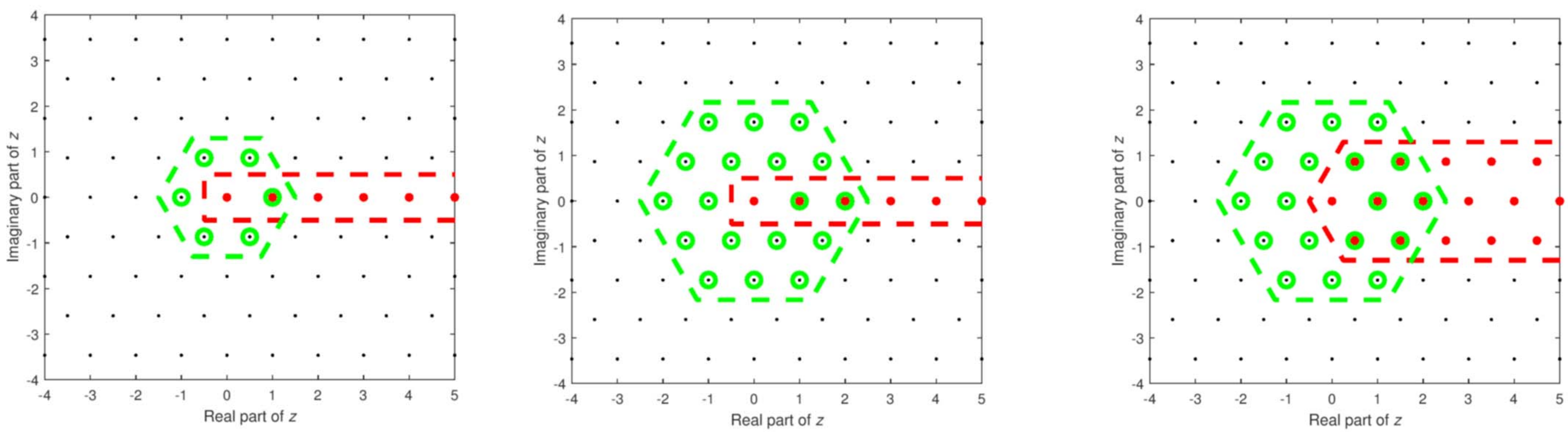
Non-periodic cases:

Examples of combinations of multi-line TR sums with end correction stencils.

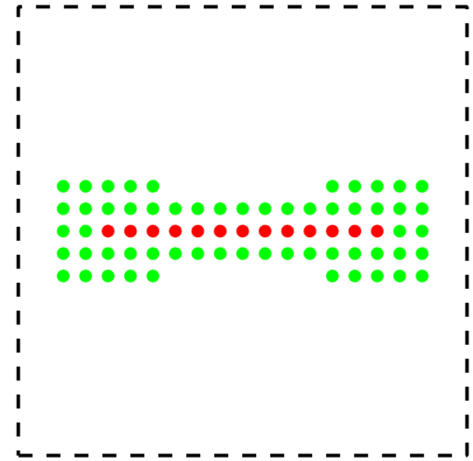
Cartesian grids:



Hexagonal grids:



Examples of FD stencil weights, Cartesian grid: 3-line TR with 5x5 end correction stencils



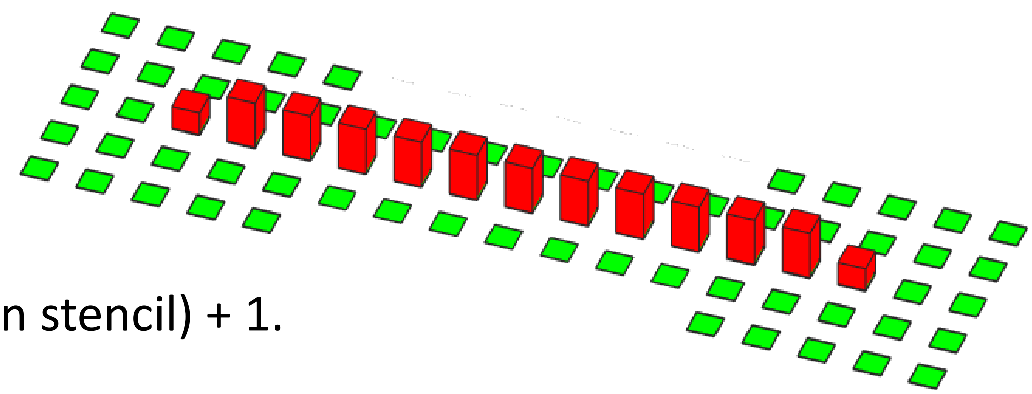
Weigh together TR over integration interval as in periodic case.

5-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

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

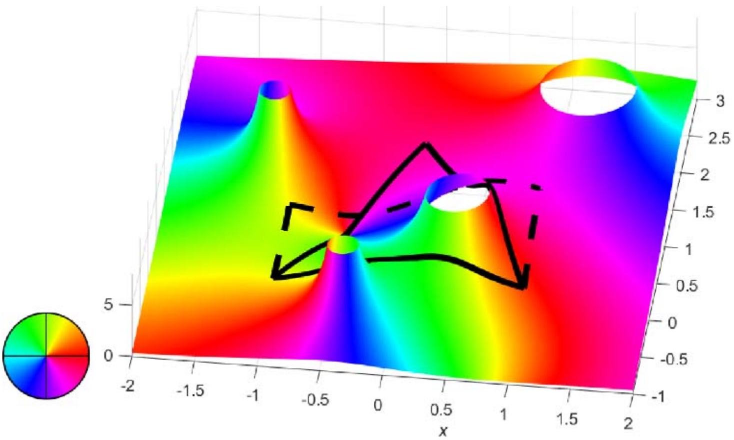


Accuracy $O(h^p)$ where p = (number of nodes in stencil) + 1.

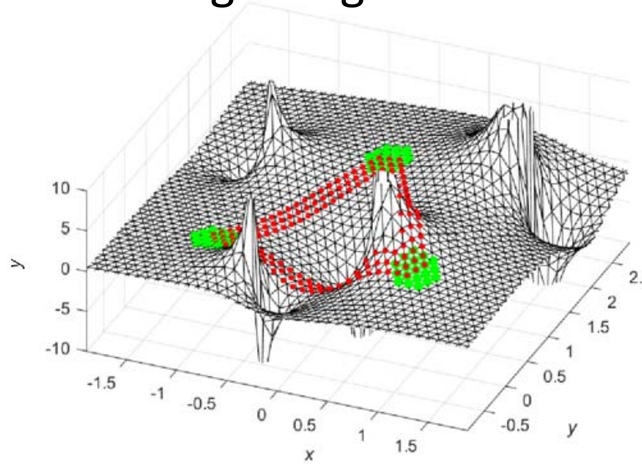
All weights are shown coefficients times h (step length in any direction in the complex plane)
Weights that are not part of the standard 1-line TR are vanishingly small.

Test problem with closed contours:

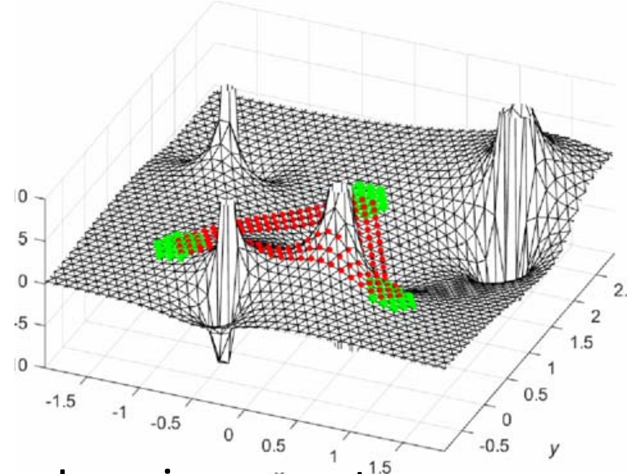
Hexagonal grid with $h = 0.1$



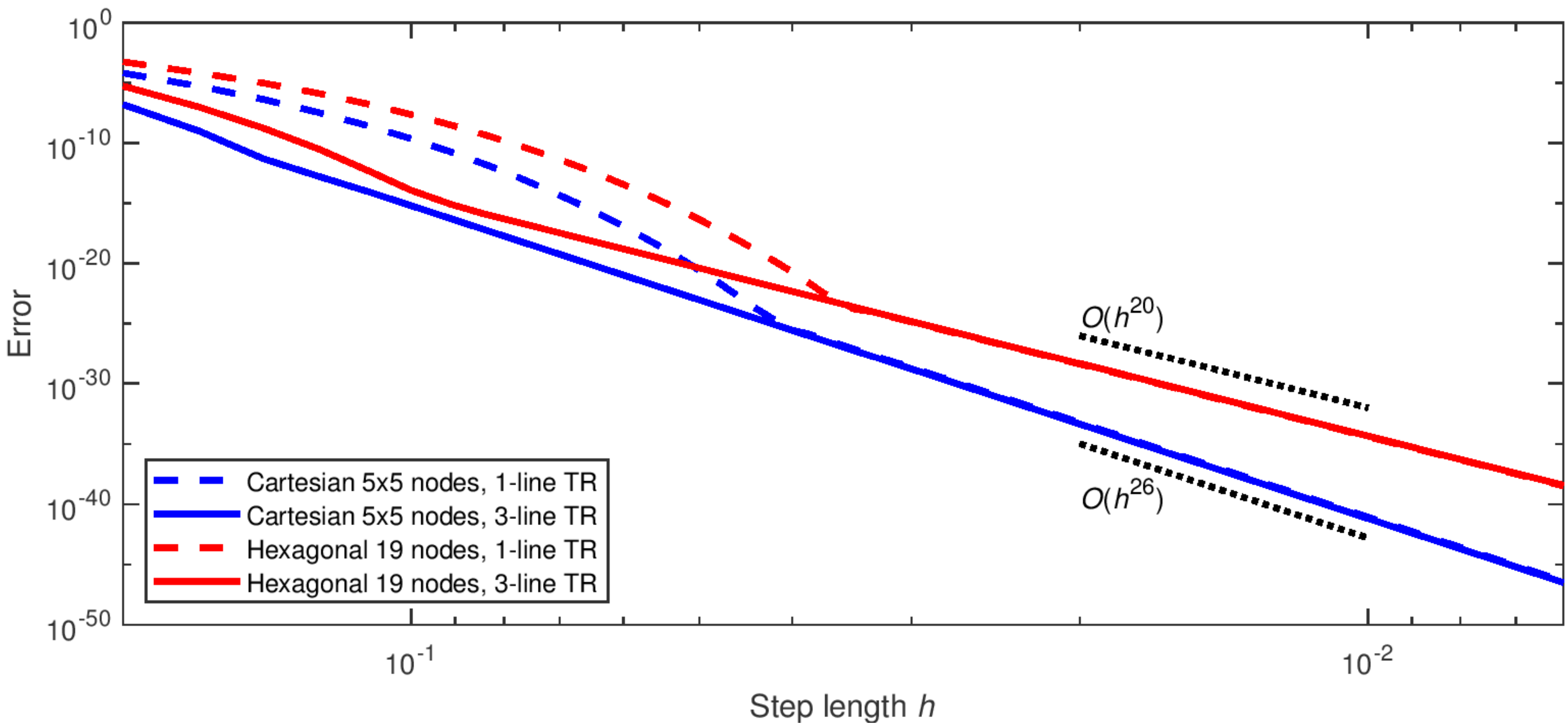
Magnitude and phase



Real part



Imaginary part

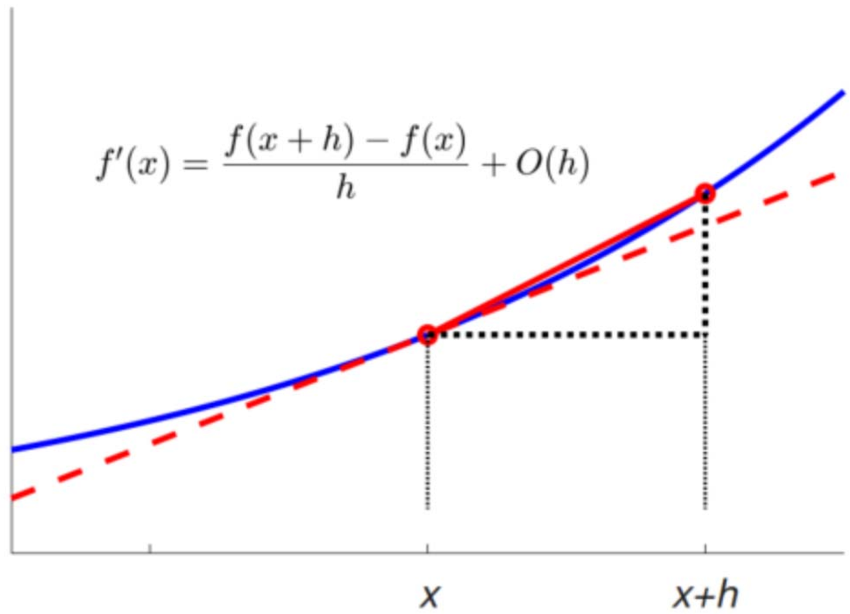


Regular derivatives:

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: $(J^n f)(x) = \dfrac{1}{(n-1)!}\int_0^x (x-t)^{n-1} f(f)dt$

Derivatives of x^m :

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

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 $n = 1/2$

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

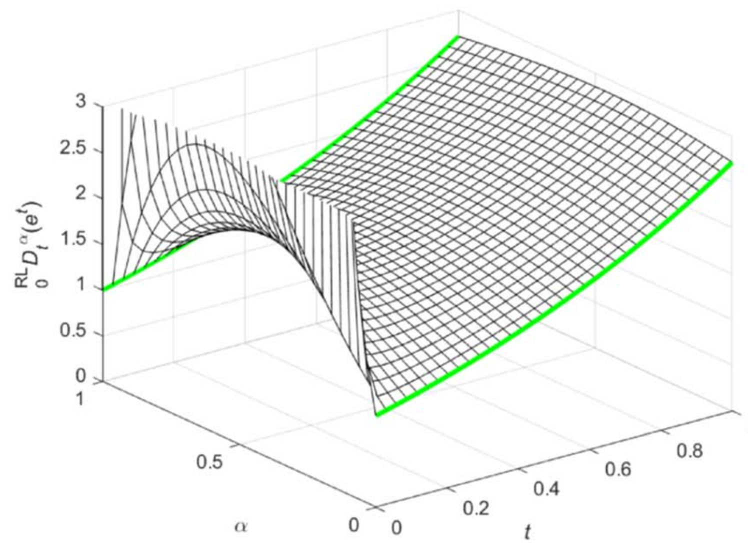
$$ {}_{0}^{C}D_t^{\alpha} f(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t \frac{\frac{d^n}{d\tau^n} f(\tau)}{(t-\tau)^{\alpha+1-n}} d\tau, \qquad n-1<\alpha<n $$

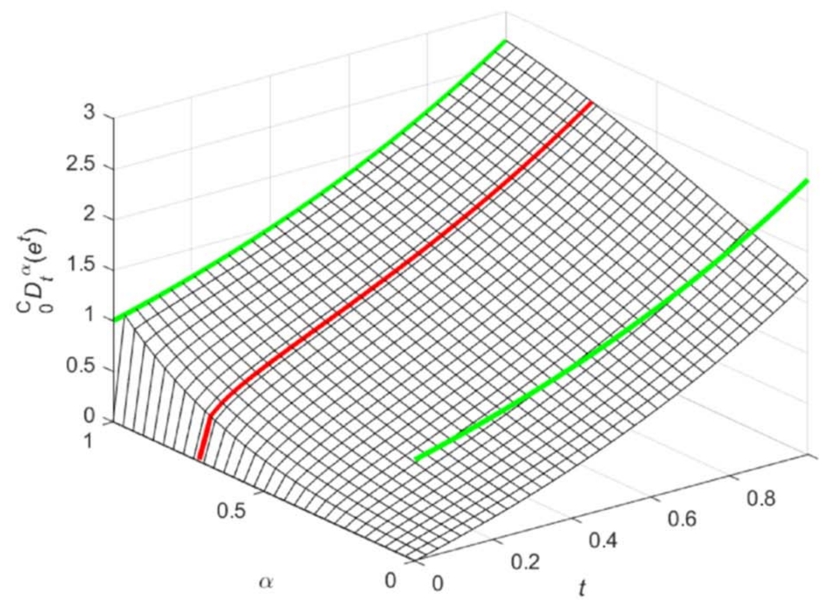
- For m integer $D^{\alpha+m} f(t) = D^{\alpha} D^m f(t)$
- D(constant) = 0
- Solving fractional ODEs requires easy initial conditions ICs

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'

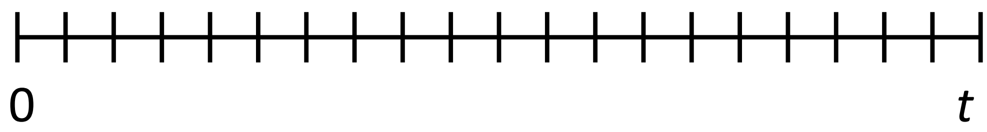
  ii. Fractional in space, $u_t = D^{\alpha}{}_{x}\, u$ with $\alpha \approx 2$, often represents better various 'anomalous' diffusion processes (typically with 'base point' on each side).

- 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

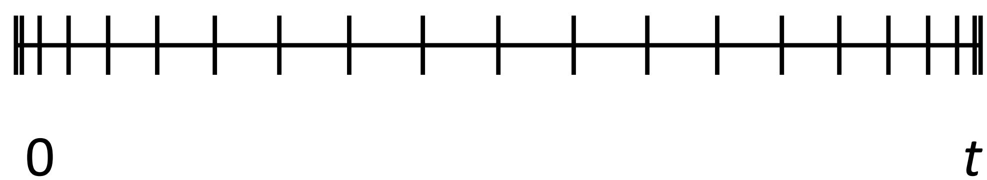


Grünwald-Letnikov formula: (1868)

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

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 impractible in time for fractional order ODEs / PDEs.

Apply complex plane integration approach to fractional derivative calculations

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

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.

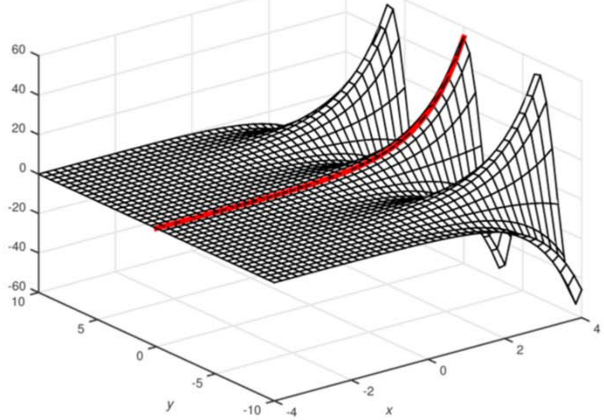
Procedure: Follow grid lines with TR and end correct wit 5x5 stencils at base point, evaluation point, and at any path corner.

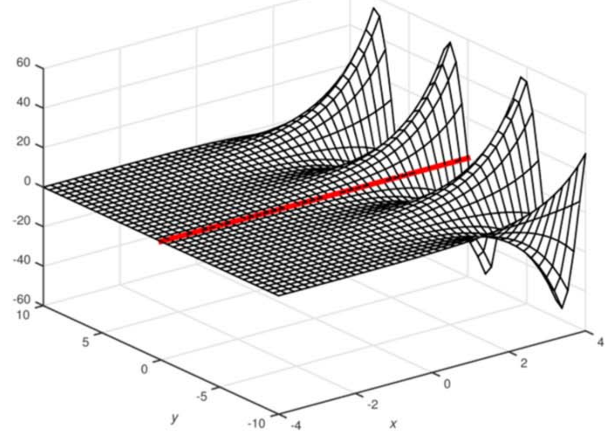
Fractional derivative illustrations:

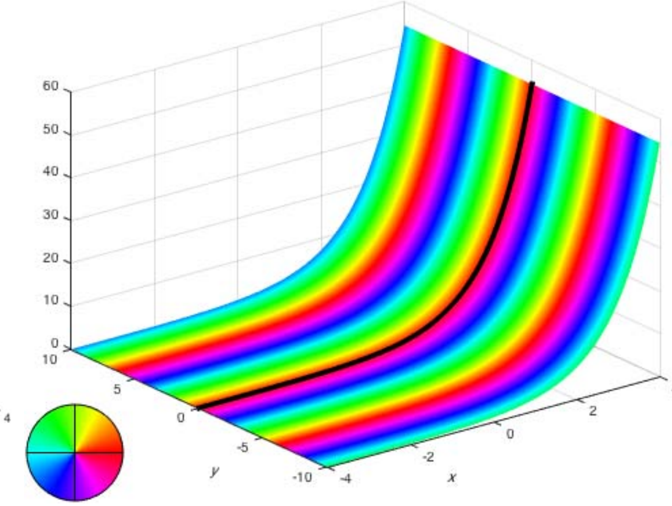
$f(z) = e^{z}$

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

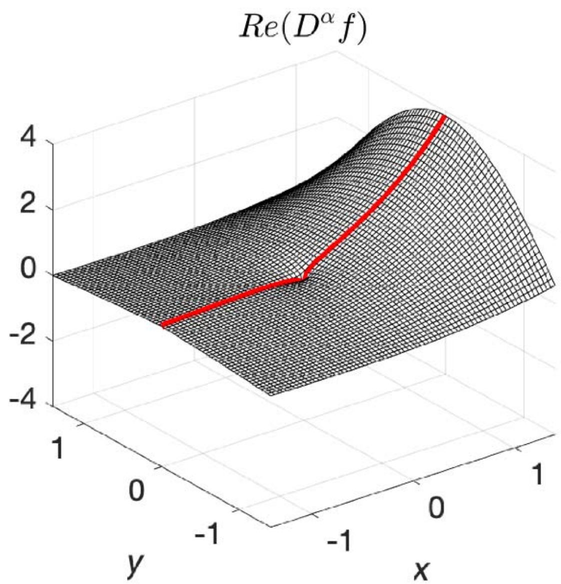
Function in complex plane:

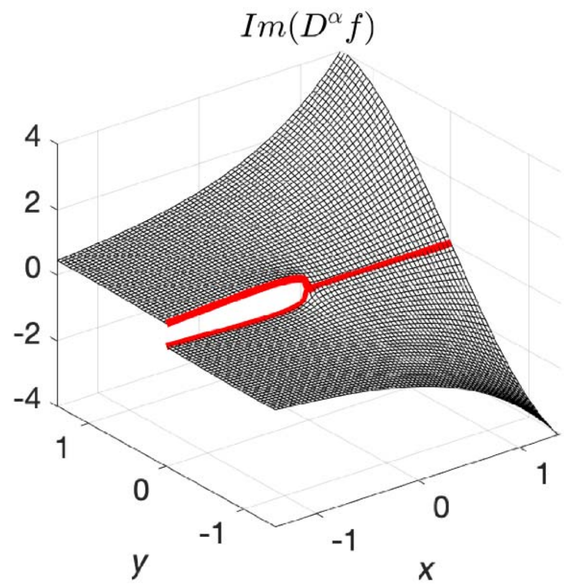


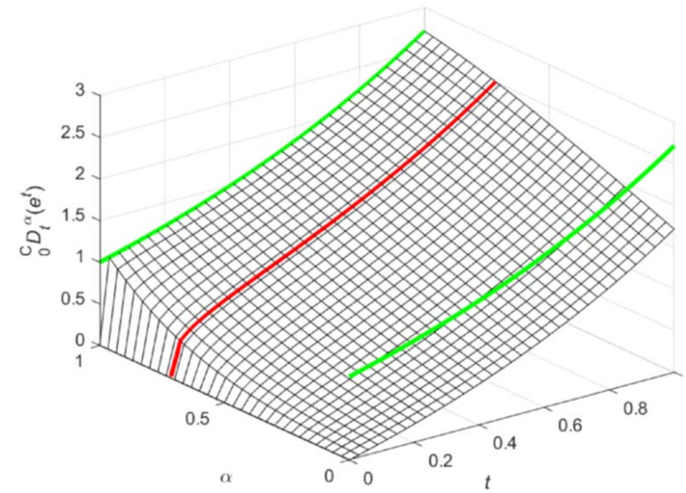




Fractional derivative, shown in the case of α = 5/7

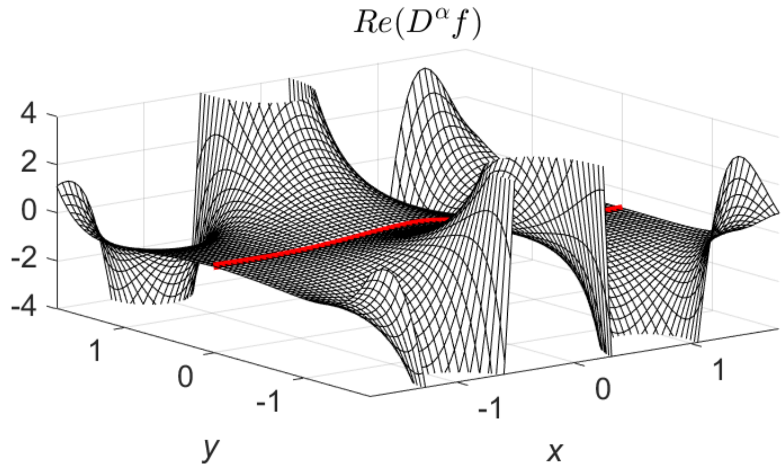


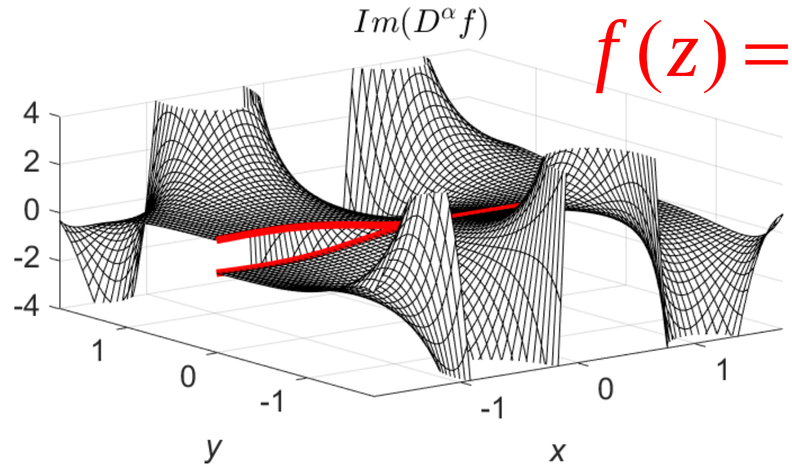




Exact: $$D^{\alpha} e^{z} = e^{z}\left(1 - \frac{\Gamma(1-\alpha, z)}{\Gamma(1-\alpha)}\right)$$

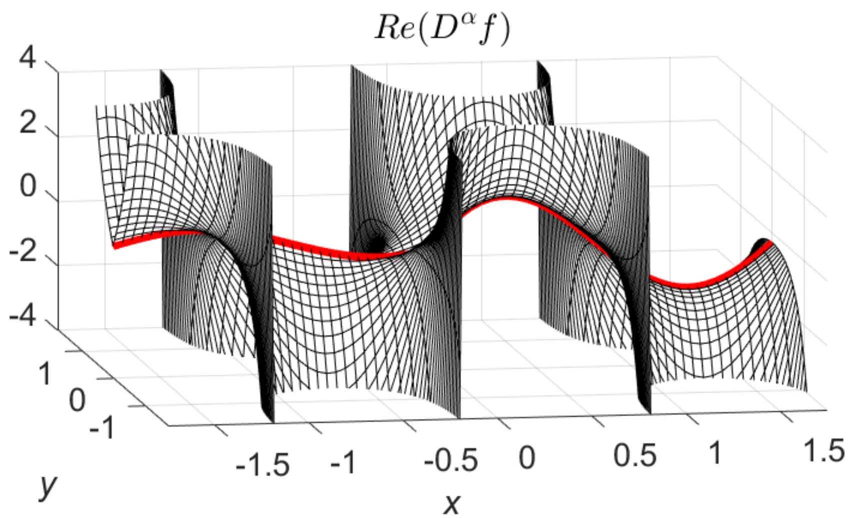
$$f(z) = e^{-z^2}$$

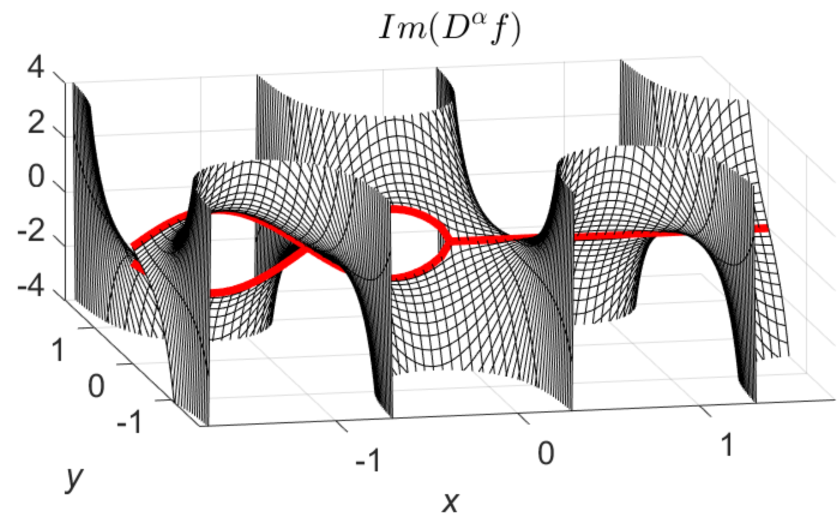




$$D^{1/3} e^{-z^2} = -\frac{9z^{5/3}}{5\Gamma(2/3)} \, {}_2F_2\left(1, \tfrac{3}{2}; \tfrac{4}{3}, \tfrac{11}{6}; -z^2\right)$$

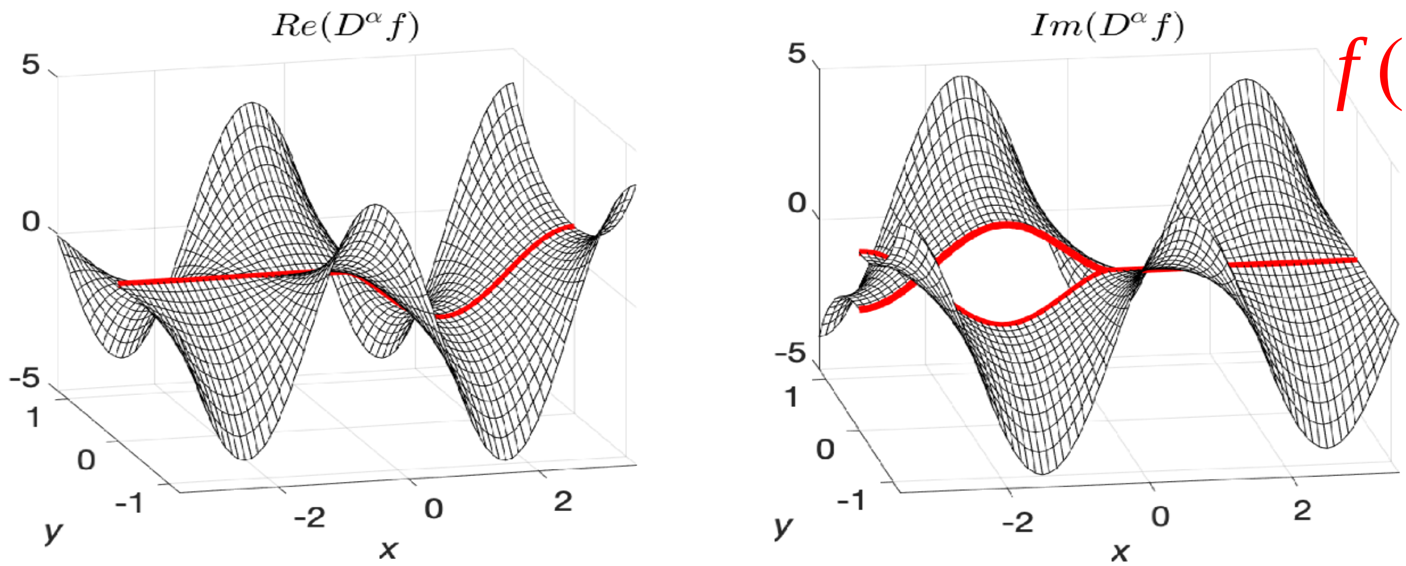
$$f(z) = \sin \pi z$$





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

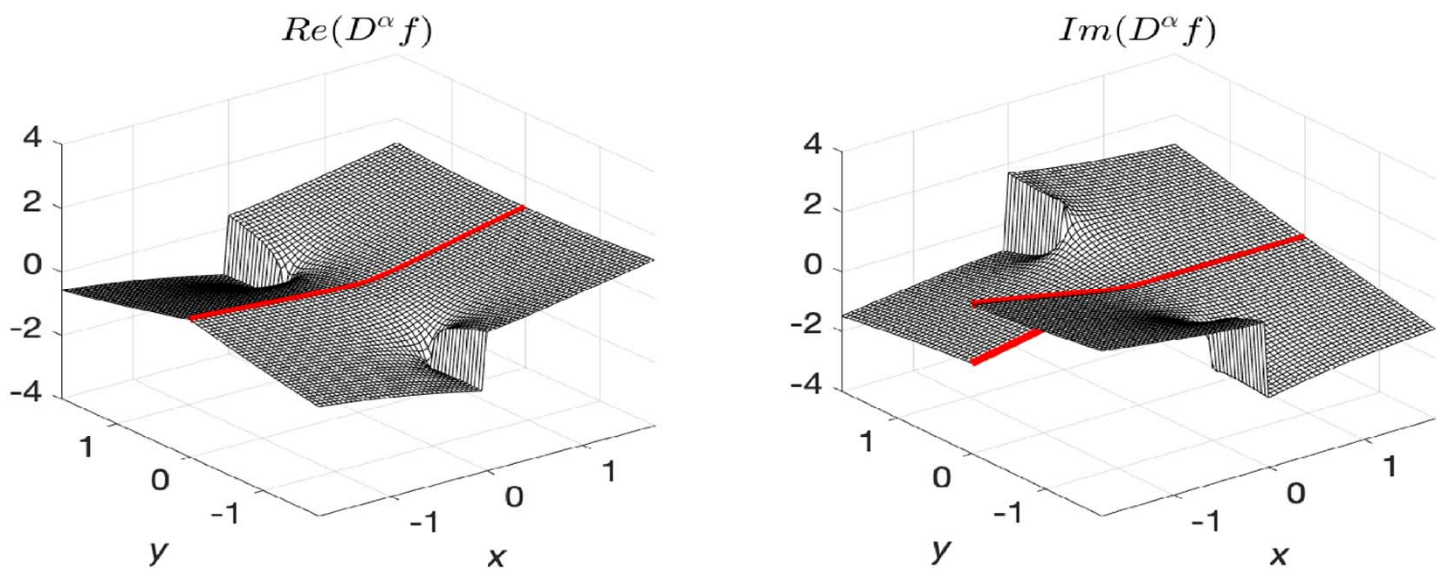
$$f(z) = \cos\left(\tfrac{\pi}{2} z\right)$$



$$D^{1/2} \cos\left(\tfrac{\pi}{2} z\right) = \sqrt{\pi}\left(\cos\left(\tfrac{\pi}{2} z\right) S(\sqrt{z}) - \sin\left(\tfrac{\pi}{2} z\right) C(\sqrt{z})\right)$$

where $S(z)$ and $C(z)$ are the Fresnel sine and cosine functions

$$f(z) = \sqrt{1+z^2}$$



$$D^{2/5}\sqrt{1+z^2} = \frac{25\, z^{8/5}}{24\Gamma(3/5)}\; {}_3F_2\left(\tfrac{1}{2}, 1, \tfrac{3}{2}; \tfrac{13}{10}, \tfrac{9}{5}; -z^2\right)$$

Some conclusions

Regular derivatives and integrals:

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

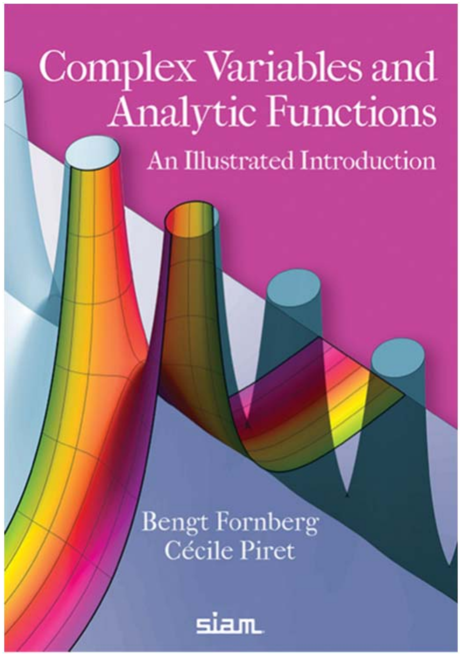
Fractional derivatives:

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

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 (especially hypergeometric) functions. For example:

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



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