Computing Fractional Derivatives of Analytic Functions

Bengt Fornberg University of Colorado, Boulder,
Department of Applied Mathematics

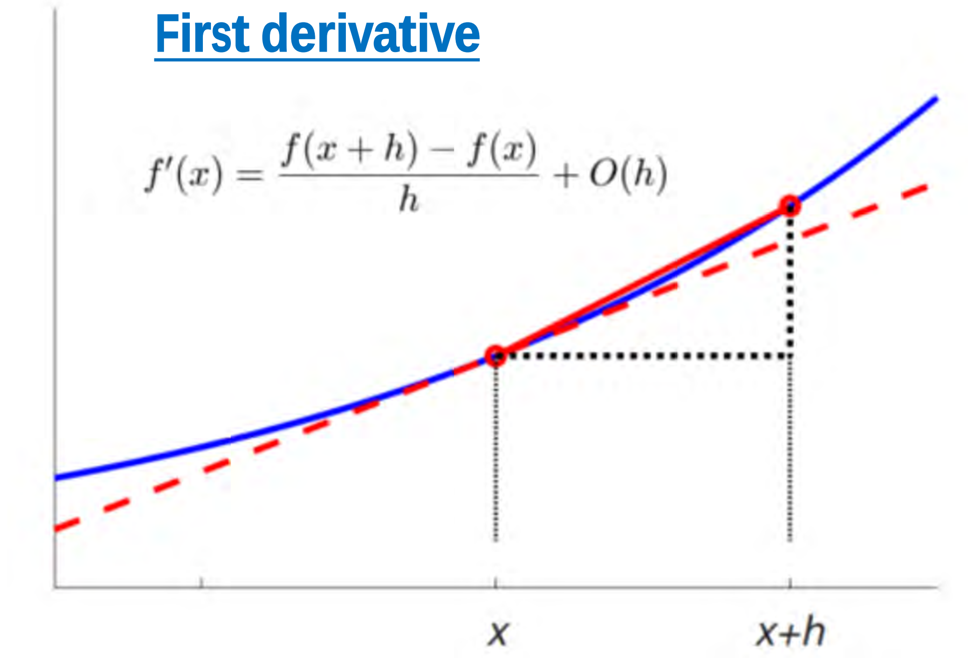
in collaboration with

Cécile Piret
Austin Higgins
Michigan Technological University, Houghton, MI.
Department of Mathematical Sciences

Outline of this presentation

- Introduction to Fractional Derivatives (5 slides)
- Background on analytic functions, (5 slides)
  FD formulas in the complex plane for regular derivatives,
  Grid-based contour integration
- Application of contour integration to fractional derivatives (1 slide)
- Illustrations of fractional derivatives (3 slides)
- Conclusions, future opportunities (1 slide)

Regular derivatives



Origin of Calculus

Gregory (1670)

Leibniz (1684), Newton (1687)

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

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

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

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 versions belong to a two-parameter family.

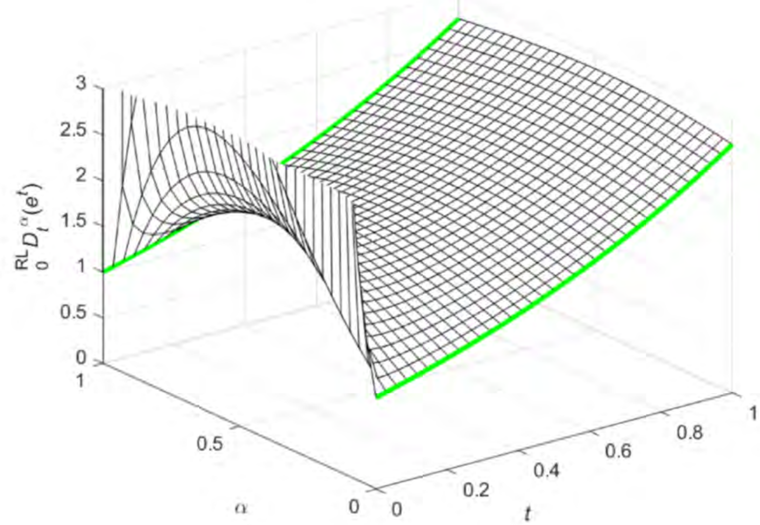
Two most commonly used types of fractional derivatives

Riemann-Liouville (1832, 1847):

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

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

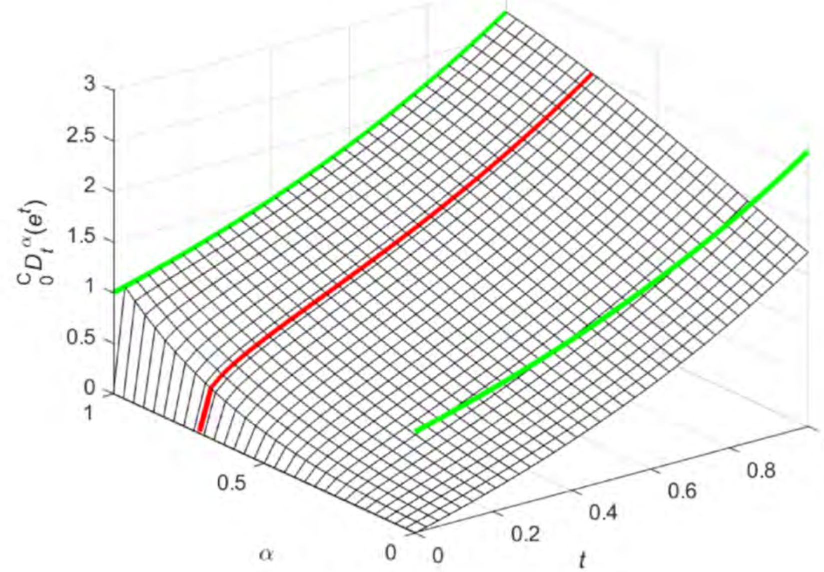
Derivative of e^t



Caputo (1967):

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

- For m integer $D^{\alpha+m} f(t) = D^{\alpha} D^m f(t)$
- D(constant) = 0
- Solving fract. ODEs by Laplace transform, easy ICs



Note also:

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

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'

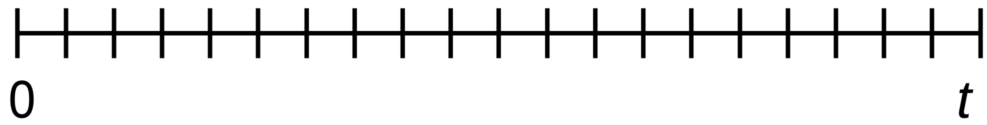
ii. Fractional in space, $u_t = D^\alpha{}_x u$ with $\alpha \approx 2$, often represents better various 'anomalous' diffusion processes (typically with 'base point' on each side).

- 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

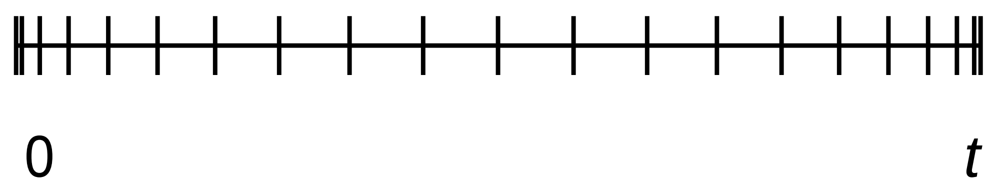


Grünwald-Letnikov formula: (1868)

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

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.

Analytic functions

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 then 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 of analyticity:

- No distinction between $\frac{\partial f}{\partial x}$ and $\frac{\partial f}{\partial y}$,
- FD formulas in the complex *x*,*y*-plane, applied to analytic functions become vastly more efficient / accurate than classical FD formulas.
- Cauchy's integral formula $f^{(k)}(z_0) = \frac{k!}{2\pi i} \oint_{\Gamma} \frac{f(z)}{(z-z_0)^{k+1}} dz \,, \; k = 0,1,2,\ldots$

  Accuracy does not depend on how close the contour Γ is to z_0.

- *f*(*z*) once differentiable implies *f*(*z*) infinitaly many times differentiable
- If *f*(*z*) is known along any curve segment, it is known for all *z*.

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 $O(h^{\{\text{number of stencil points}\} - p})$

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

Extremely high accuracies already for very small stencils

The Euler-Maclaurin formula

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

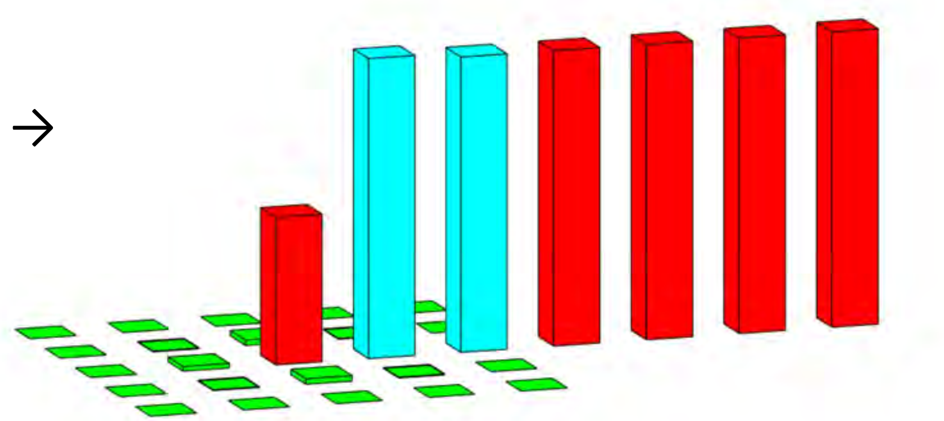
Trapezoidal rule (TR) approximation:

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

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

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

- Magnitude of correction weights extremely small also in 5x5 stencil case →→→



- Accuracy order one above the number of stencil points (in the 5x5 case $O(h^{24})$)
- 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.

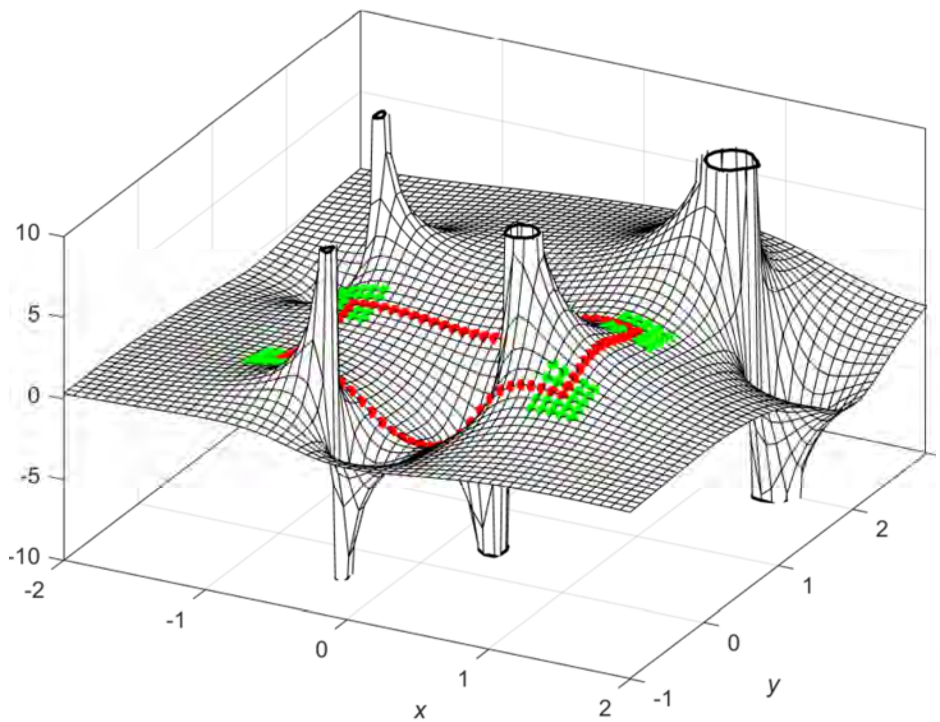
The order of accuracy of the resulting quadrature approach will match the number of equated coefficients.

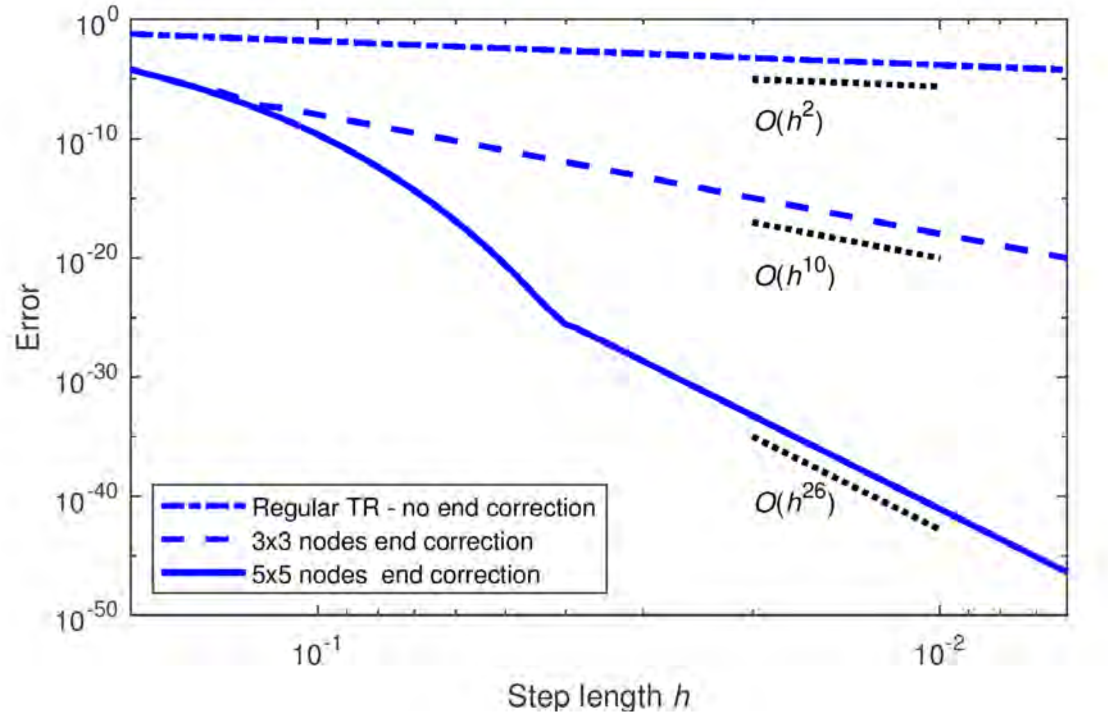
For this method, we don't even need to know that the Euler-Maclaurin formula exists
(will be utilized for fractional derivative generlizations)

Contour integration in the complex plane

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

Log-log plot of error





- The accuracy needed for a reasonably resolved functional display (above, left) is about the same as needed for typical double precision $O(10^{-16})$ contour integral accuracy (i.e., no additional function evaluations are needed beyond what the grid already contains).

- No apparent ill effect of singularities very near to a FD stencils.

- Loss of accuracy seen for 5x5, large *h*, comes from TR and can be corrected for.

Apply this integration approach to fractional derivative calculations

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 correction stencils also for the singular end point $\tau = z$ of the integrand.

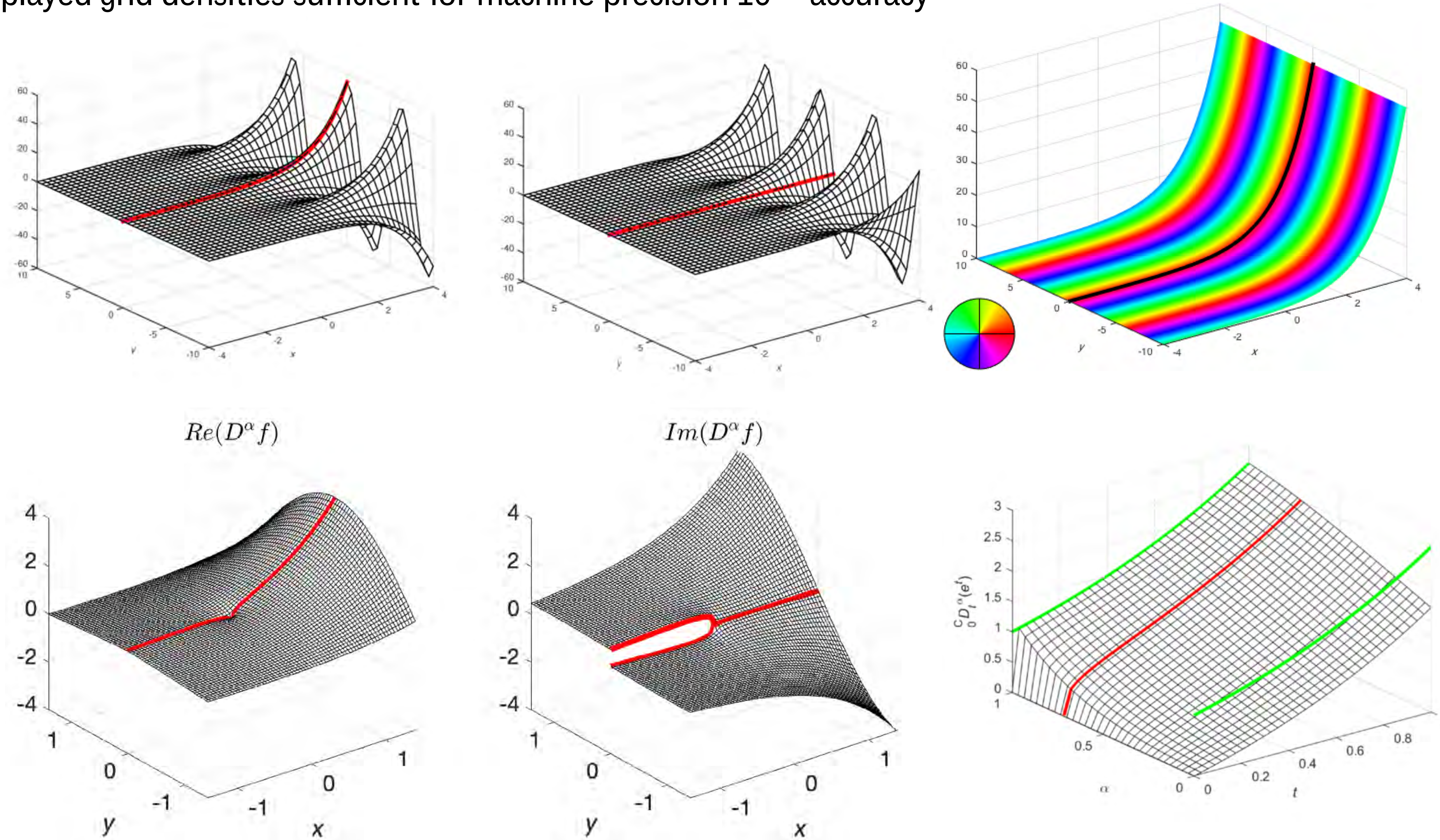
An additional technicality is needed when the evaluation point z is close to the base point 0.

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:

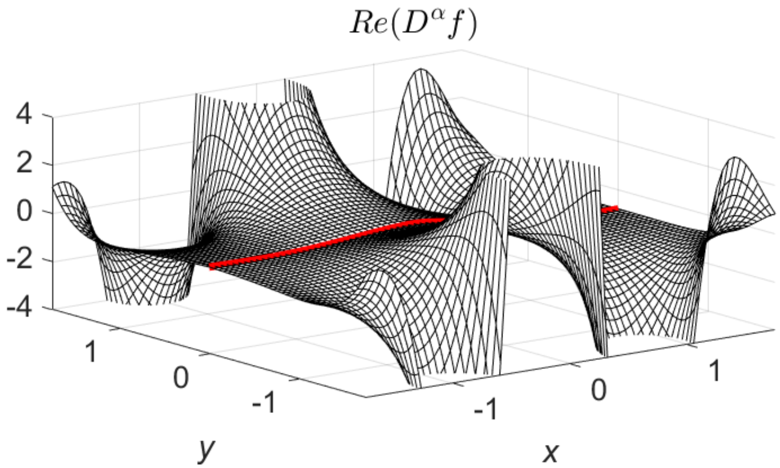
Displayed grid densities sufficient for machine precision 10^{-16} accuracy

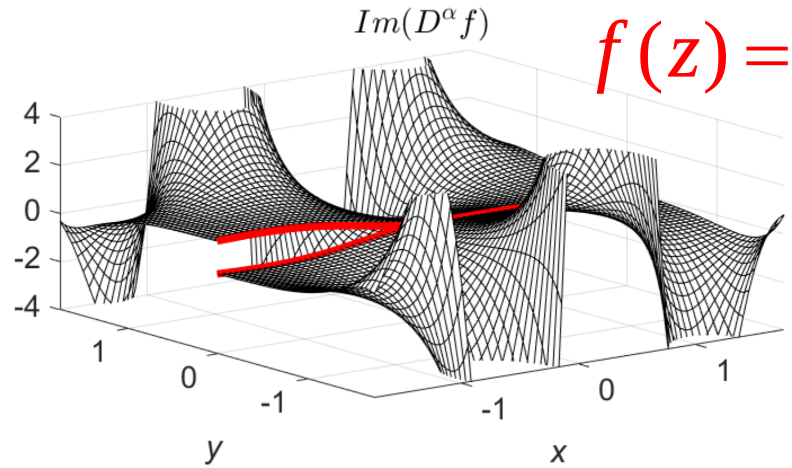
$$f(z) = e^{z}$$



Exact: $D^{\alpha} e^{z} = e^{z}\left(1 - \dfrac{\Gamma(1-\alpha, z)}{\Gamma(1-\alpha)}\right)$, shown in the case of α = 5/7.

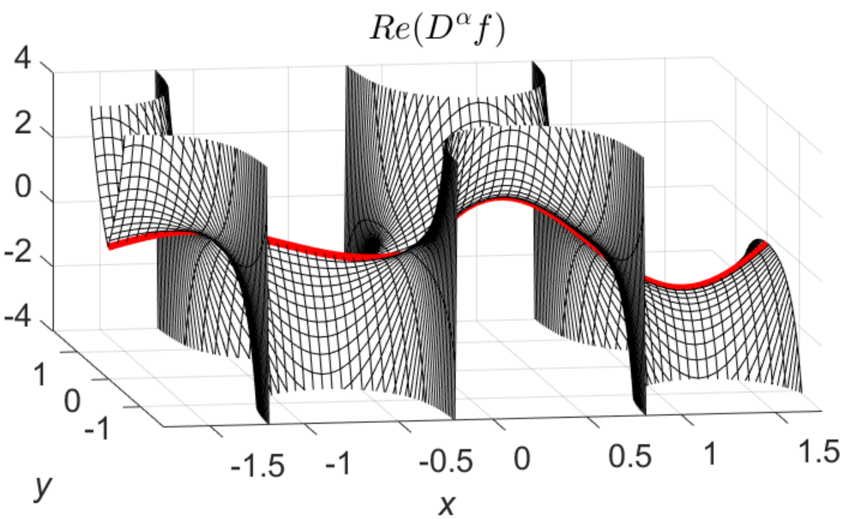
$$f(z) = e^{-z^2}$$

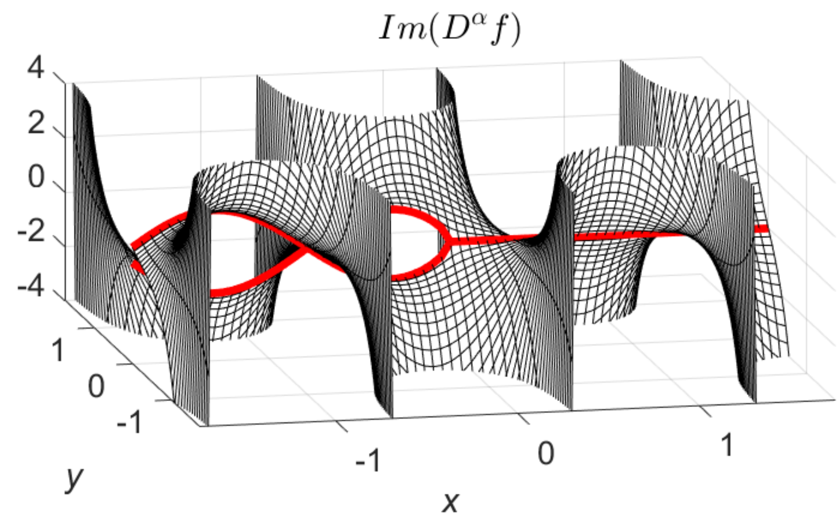




$$D^{1/3}e^{-z^2} = -\frac{9z^{5/3}}{5\Gamma(2/3)}\;{}_2F_2\left(1,\tfrac{3}{2};\tfrac{4}{3},\tfrac{11}{6};-z^2\right)$$

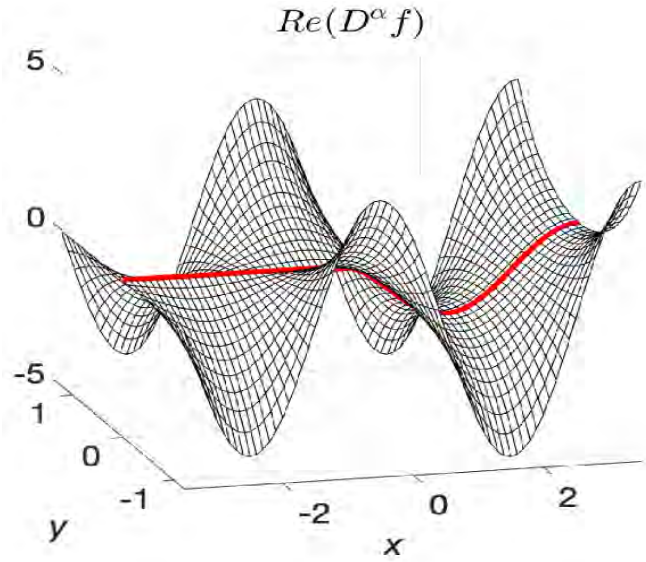
$$f(z) = \sin \pi z$$

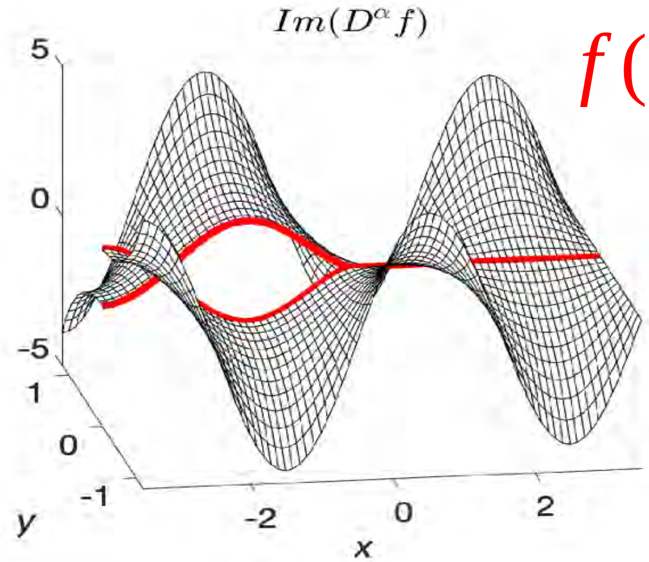




$$D^{\pi/8}\sin \pi z = \frac{\pi\, z^{1-\pi/8}}{\Gamma(1-\frac{\pi}{8})}\;{}_1F_2\left(1;1-\tfrac{\pi}{8},\tfrac{3}{2}-\tfrac{\pi}{16};-\tfrac{\pi^2 z^2}{4}\right)$$

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

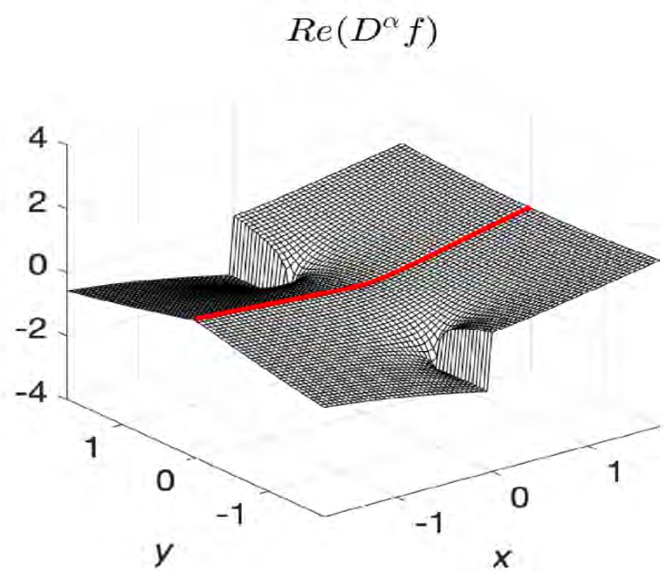


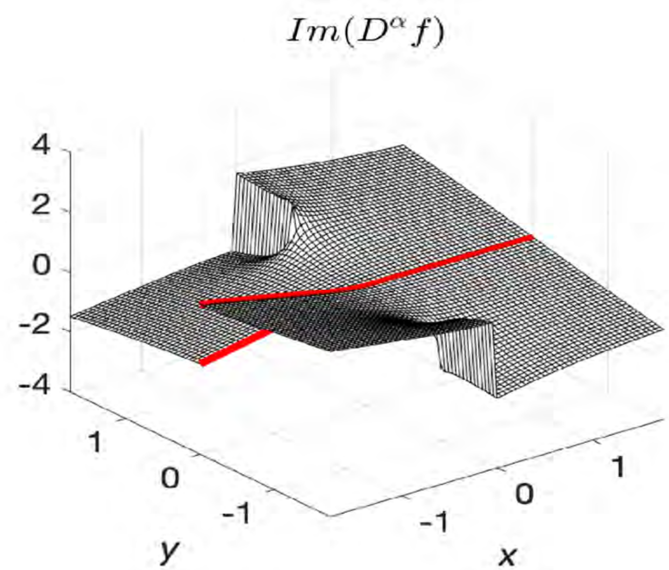


$$D^{1/2} \cos\left(\tfrac{\pi}{2} z\right) = \sqrt{\pi}\left(\cos\left(\tfrac{\pi}{2} z\right) S(\sqrt{z}) - \sin\left(\tfrac{\pi}{2} z\right) C(\sqrt{z})\right)$$

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

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





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

Main conclusion

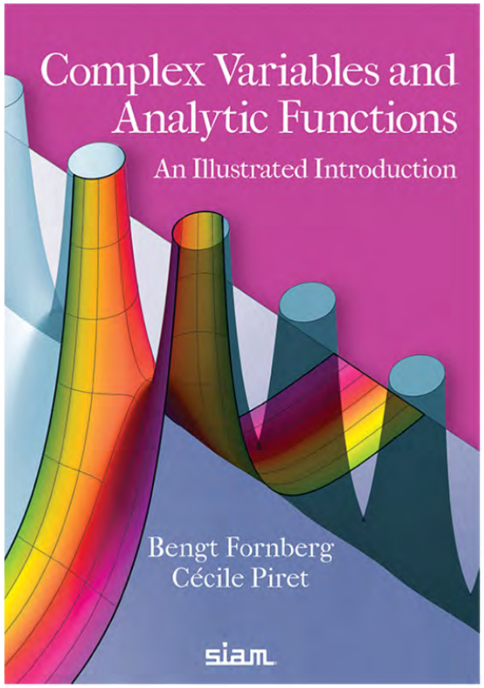
- Fractional derivatives can be computed to machine precision accuracy using grids with density comparable to what is needed for typical functional displays

Future opportunities (currently being pursued)

- Some special functions are the fractional derivative of elementary functions. This can be utilized this to simplify their numerical evaluation in the complex plane

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

- Develop a similar end-correction algorithm that uses data only along the real axis, within (or also outside) the interval [0,t].



References:

B.F., *Contour integrals of analytic functions given on a grid in the complex plane*, IMA J. Num. Anal. (2021).
B.F., *Complex plane finite difference formulas*, Numerical Algorithms (2022).
B.F. and C. Piret, *Complex Variables and Analytic functions: An Illustrated Introduction*, SIAM (2020) → → →
B.F. and C. Piret, *Computation of fractional derivatives of analytic functions*, submitted.
A. Higgins, *Numerical computations of fractional derivatives of analytic functions*, submitted.