Finite Difference Formulas in the Complex Plane

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Some FD background

A few historical notes

c 1592	Jost Bürgi (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	$\frac{4}{5}$	$-\frac{1}{5}$	$\frac{4}{105}$	$-\frac{1}{280}$
	↓	↓	↓	↓	↓	↓	↓	↓	↓
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	$-\frac{2}{4^2}$	$\frac{2}{3^3}$	$-\frac{2}{2^2}$	$\frac{2}{1^2}$	$-\frac{\pi^2}{3}$	$\frac{2}{1^2}$	$-\frac{2}{2^2}$	$\frac{2}{3^3}$	$-\frac{2}{4^2}$

Pseudospectral (PS) limit of (formally) infinite order of accuracy

If data is periodic, one can repeat it indefinitely, and then apply an infinitely wide FD limit stencil.

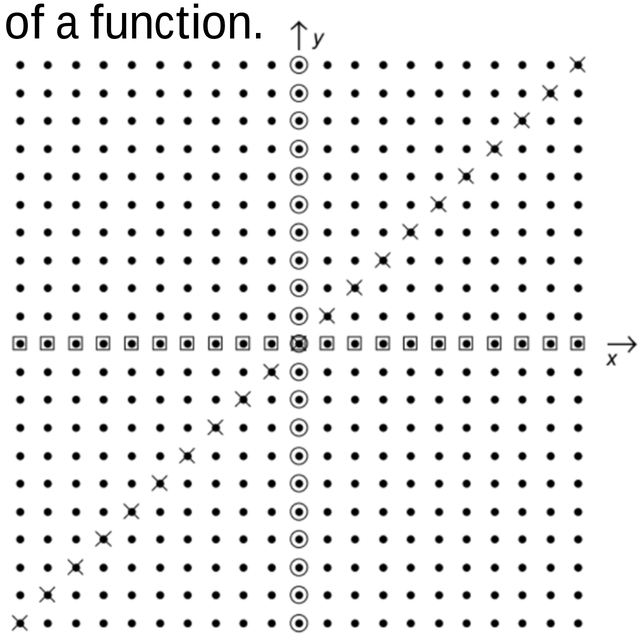
Theorem: The result becomes identical to having done an FFT on data, and then analytically having differentiated the obtained trigonometric interpolant.

PS methods can be highly efficient, but have two main flaws:

1. Approximations are not 'local'

1st derivative weights	$\cdots$	$\frac{1}{4}$	$-\frac{1}{3}$	$\frac{1}{2}$	-1	0	1	$-\frac{1}{2}$	$\frac{1}{3}$	$-\frac{1}{4}$	$\cdots$
2nd derivative weights	$\cdots$	$-\frac{2}{4^2}$	$\frac{2}{3^2}$	$-\frac{2}{2^2}$	$\frac{2}{1^2}$	$-\frac{\pi^2}{3}$	$\frac{2}{1^2}$	$-\frac{2}{2^2}$	$\frac{2}{3^2}$	$-\frac{2}{4^2}$	$\cdots$
etc.											

Derivatives should be a 'local' property of a function.



2. Anisotropy

Compare approximations for

$$\frac{\partial}{\partial x}, \quad \frac{\partial}{\partial y}, \quad \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\right).$$

Last case is a derivative in a direction along which no data has been utilized

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

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

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

......

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

......

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

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

......

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

Examples of applications: The Euler-Maclaurin formula

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

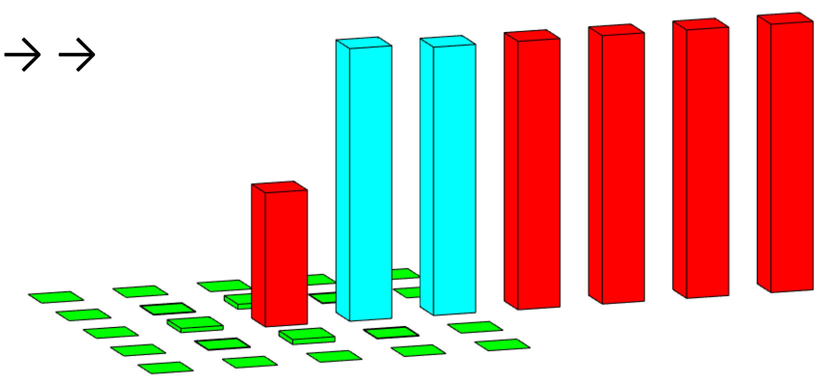
Trapezoidal rule (TR) approximation:

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

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

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

- Magnitude of weights in 5x5 stencil case → → →
  No danger of numerical cancellations.

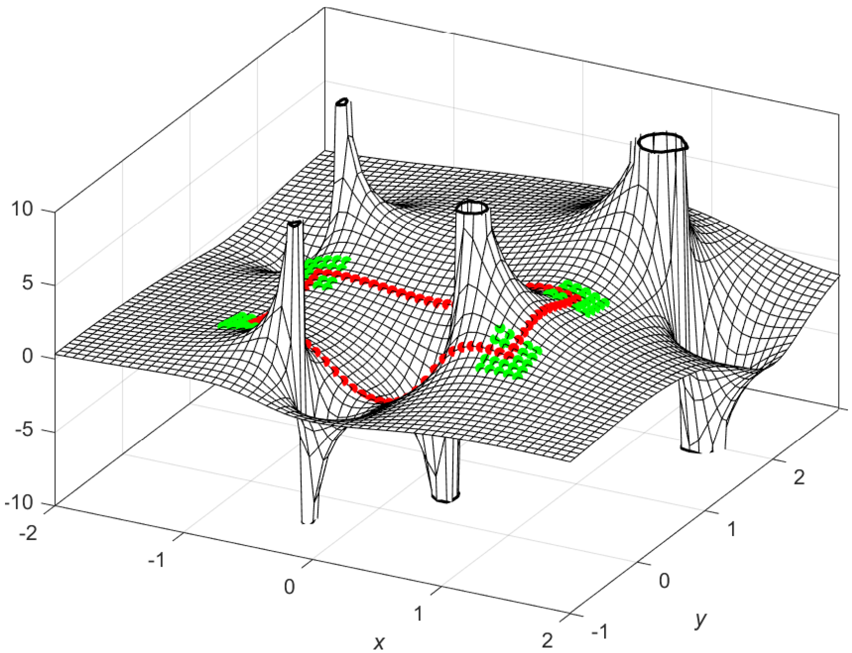


- Accuracy order one above the number of stencil points

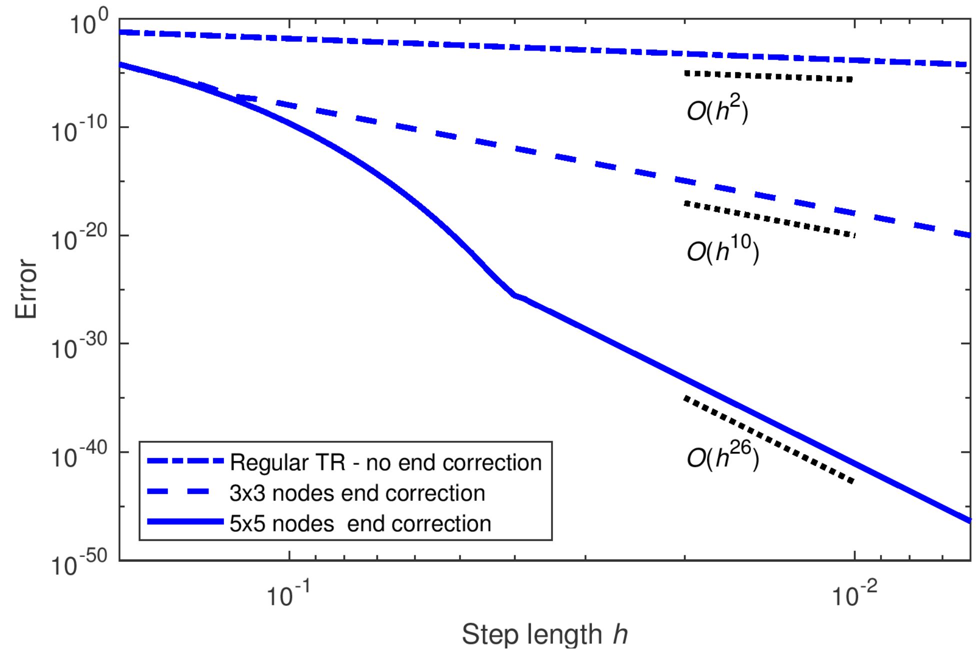
- For finite interval, matching expansion at the opposite end

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.

Numerical analytic continuation

Analytic continuation: Circle-chain theorem: Useful for theoretical insights only; Several more practical continuation options are available

Numerical continuation: FD formulas can provide a practical numerical approach

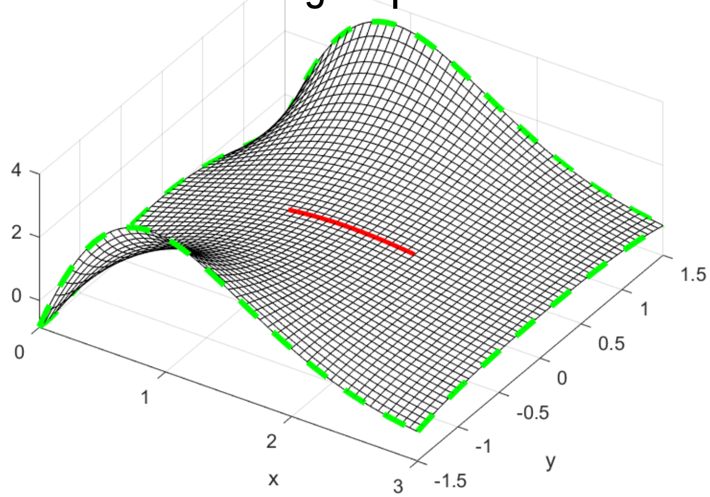
Recall $f^{(8)}(0) = \frac{504}{h^8}\begin{bmatrix} 1 & 4 & 1 \\ 4 & -20 & 4 \\ 1 & 4 & 1 \end{bmatrix} f + O(h^1)$; can be expressed as $\begin{bmatrix} 1 & 4 & 1 \\ 4 & -20 & 4 \\ 1 & 4 & 1 \end{bmatrix} f = 0 + O(h^8)$

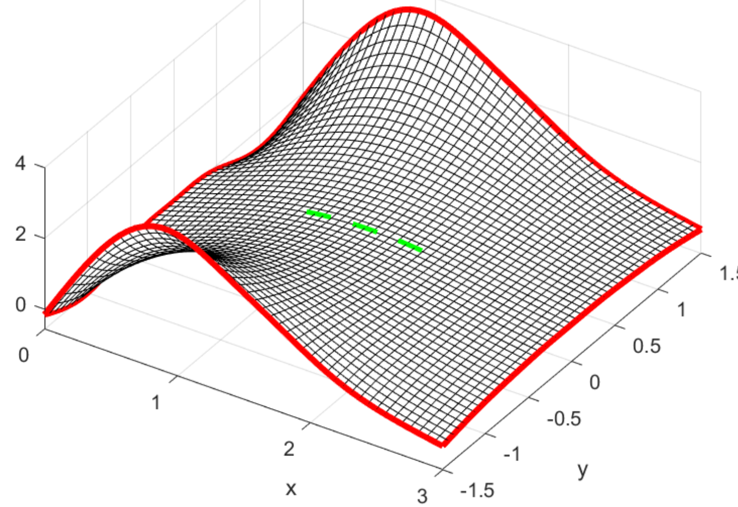
Example:

Function Re[1/Γ(z)] given around edge of [0,3]x[-1.5,1.5], then solved over interior by applying the 3x3 stencil at all interior grid points

In reverse: Function Re[1/Γ(z)] now given only at The 17 grid points along [0,1]. Then enforce:

- Stencil at all interior points,
- Exact values at 17 grid points along [0,1]
- Least square minimize [1 -2 1] around boundary





Numerical calculation of the conjugate harmonic function

The Cauchy-Riemann equations: With $f(z) = u(x,y) + i\,v(x,y)$, then $\dfrac{\partial u}{\partial x} = \dfrac{\partial v}{\partial y}$, $\dfrac{\partial u}{\partial y} = -\dfrac{\partial v}{\partial x}$.

Present task: Given $u(x,y)$ over a grid, calculate the matching $v(x,y)$.

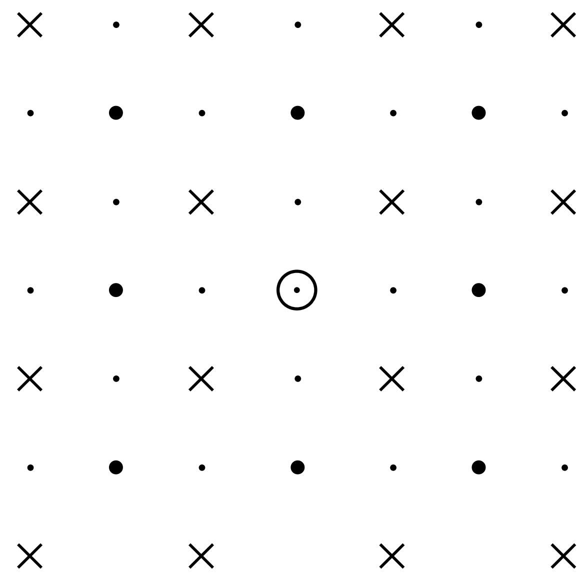
Basic FD formula:

$$\frac{1}{h}\begin{bmatrix}-1 & 1\end{bmatrix} v = \frac{1}{4h}\begin{bmatrix}-1 & -1\\ 0 & 0\\ 1 & 1\end{bmatrix} u + O(h^2)$$

More accurate version:

$$\frac{1}{h}\begin{bmatrix}-1 & 1\end{bmatrix} v = \frac{1}{h}\begin{bmatrix}-0.0010 & -0.0059 & -0.0059 & -0.0010\\ 0.0222 & 0.1666 & 0.1666 & 0.0222\\ 0.1408 & -0.2479 & -0.2479 & 0.1408\\ 0 & 0 & 0 & 0\\ -0.1408 & 0.2479 & 0.2479 & -0.1408\\ -0.0222 & -0.1666 & -0.1666 & -0.0222\\ 0.0010 & 0.0059 & 0.0059 & 0.0010\end{bmatrix} u + O(h^{12})$$

Interpolation to a denser grid



For analytic (and harmonic) functions, the small stencil below is 4th order accurate:

$$f(\odot) = \frac{1}{4}\begin{bmatrix} 1 & & 1 \\ & \odot & \\ 1 & & 1 \end{bmatrix} f + O(h^4)$$

For larger stencils, the order becomes the same as the total number of nodes; for example:

$$f(\odot) = \frac{1}{106496}\begin{bmatrix} -25 & 162-459i & & 162+459i & -25 \\ 162+459i & 26325 & & 26325 & 162-459i \\ & & \odot & & \\ 162-459i & 26325 & & 26325 & 162+459i \\ -25 & 162+459i & & 162-459i & -25 \end{bmatrix} f + O(h^{16})$$

Coupling between real and imaginary parts can be removed with slight drop in order

$$f(\odot) = \frac{81}{1024}\begin{bmatrix} 13/18 & 1 & & 1 & 13/18 \\ 1 & 1 & & 1 & 1 \\ & & \odot & & \\ 1 & 1 & & 1 & 1 \\ 13/18 & 1 & & 1 & 13/18 \end{bmatrix} f + O(h^{12})$$

Pseudospectral (PS) limit of increasing orders / stencil sizes

Recall: 1st derivative; the weights in PS limit are: $\cdots \; \frac{1}{4} \; -\frac{1}{3} \; \frac{1}{2} \; -1 \; 0 \; 1 \; -\frac{1}{2} \; \frac{1}{3} \; -\frac{1}{4} \; \cdots$

Problematic, since derivatives should be a 'local' property of a function.

General result (1-D real, or complex): Approximate d/dz at $z = 0$ with nodes at $z = z_k$.

By differentiating Lagrange's interpolation formula, the 1st derivative weights are:

$$w_k = -\frac{1}{z_k}\left(\frac{\left.\frac{\mathrm{d}\phi}{\mathrm{d}z}\right|_{z=0}}{\left.\frac{\mathrm{d}\phi}{\mathrm{d}z}\right|_{z=z_k}}\right)$$

with *node polynomial* $\phi(z) = \prod_{k=1}^{N}(z - z_k)$

One node at $z = 0$, w_k weight at a different node

Regular FD: With 1-D unit-spaced nodes: $z_k = 0, \pm1, \pm2, \pm3, \ldots$

Noting: $\phi(z) = (-1)^N N! \prod_{k=1}^{N}\left(1 - \frac{z^2}{k^2}\right)$ and $\lim_{N\to\infty} \prod_{k=1}^{N}\left(1 - \frac{z^2}{k^2}\right) = \frac{\sin \pi z}{\pi z}$

shows that ($k \neq 0$) $\left(\frac{\left.\frac{\mathrm{d}\phi}{\mathrm{d}z}\right|_{z=0}}{\left.\frac{\mathrm{d}\phi}{\mathrm{d}z}\right|_{z=z_k}}\right) \to \pm 1$ and $w_k = \pm\frac{1}{k}$.

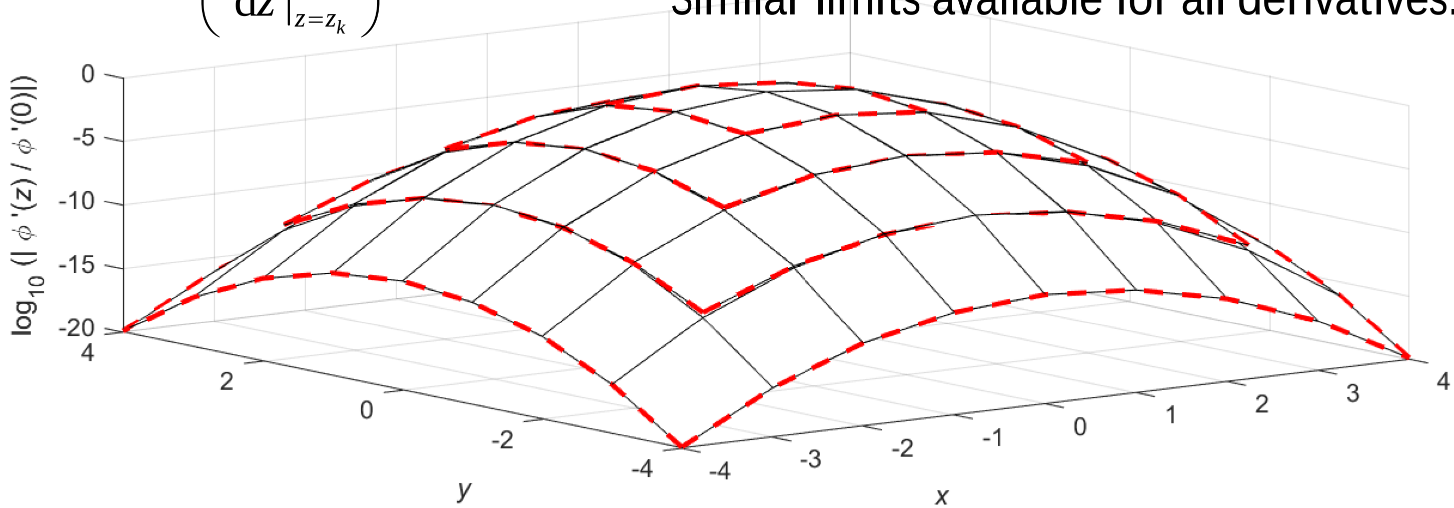
PS limit of increasing orders / stencil sizes – Complex plane case

The formula $$w_k = -\frac{1}{z_k}\left(\frac{\left.\frac{\mathrm{d}\phi}{\mathrm{dz}}\right|_{z=0}}{\left.\frac{\mathrm{d}\phi}{\mathrm{dz}}\right|_{z=z_k}}\right)$$ still holds.

Consider unit-spaced stencils: $z_k = \mu + \nu\, i, \;\; \text{with} \;\; \mu = 0, \pm 1, \pm 2, \ldots, \pm n, \quad \nu = 0, \pm 1, \pm 2, \ldots, \pm n.$

Then (for $z_k \neq 0$) $$\left(\frac{\left.\frac{\mathrm{d}\phi}{\mathrm{dz}}\right|_{z=0}}{\left.\frac{\mathrm{d}\phi}{\mathrm{dz}}\right|_{z=z_k}}\right) \to \pm\, e^{-\frac{\pi}{2}\left|z_k\right|^2}$$, so PS limit for 1st derivative $$w_k = \pm \frac{1}{z_k} e^{-\frac{\pi}{2}\left|z_k\right|^2}$$

Similar limits available for all derivatives.



The extrememly rapid decay rate of the coefficients explains why complex plane FD formulas can be applied very near to singularities with only minimal loss of accuracy.

PS limit of increasing orders of accuracy / stencil sizes

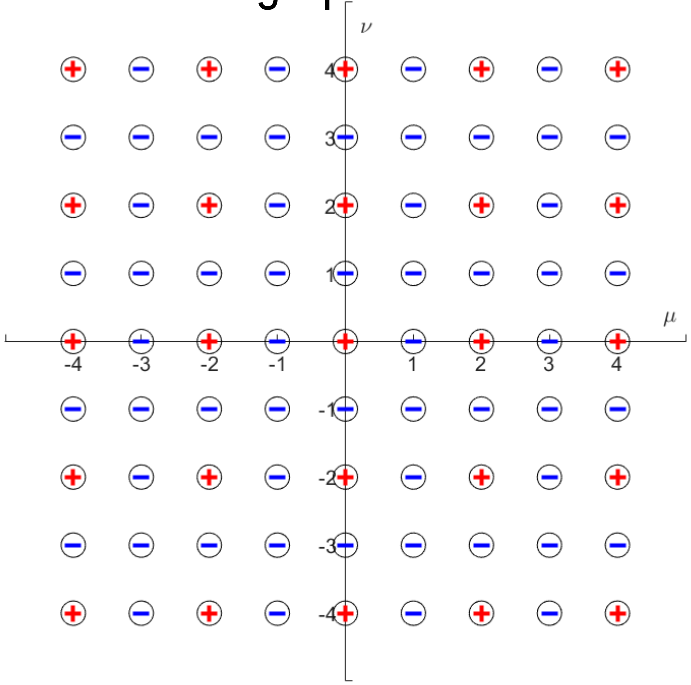
1st derivative $\quad w_k = \pm \frac{1}{z_k} e^{-\frac{\pi}{2}|z_k|^2}$

2nd derivative $\quad w_k = \pm \frac{2}{z_k^2} e^{-\frac{\pi}{2}|z_k|^2}$

3rd derivative $\quad w_k = \pm \frac{6}{z_k^3} e^{-\frac{\pi}{2}|z_k|^2}$

4th derivative $\quad w_k = \pm \frac{24}{z_k^4} e^{-\frac{\pi}{2}|z_k|^2}$

± sign pattern



For higher derivatives, get more terms with each term still of similar form

A couple of algorithms to calculate FD weights

Task: Find the optimal weights w_k at nodes z_k to approximate a linear operator L at $z = 0$. The nodes z_k are arbitrary placed (but assumed distinct).

Method 1: Solve a Vandermonde system

Require the exact result for as many powers of z as possible

$$\begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ z_1 & z_2 & z_3 & \cdots & z_N \\ z_1^2 & z_2^2 & z_3^2 & \cdots & z_N^2 \\ \vdots & \vdots & \vdots & & \vdots \\ z_1^{N-1} & z_2^{N-1} & z_3^{N-1} & \cdots & z_N^{N-1} \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_N \end{bmatrix} = \begin{bmatrix} L1\,|_{z=0} \\ Lz\,|_{z=0} \\ Lz^2\,|_{z=0} \\ \vdots \\ Lz^{N-1}\,|_{z=0} \end{bmatrix}$$

This linear system is non-singular, but is usually severely ill-conditioned.

Proof of non-singularity when the z_k are distinct:

Call the system matrix A, and rename z_N to z. Then, det(A) is a polynomial in z of degree N-1, i.e., it can have at most N-1 roots. All these roots are accounted for by $z = z_1$, $z = z_2$, ... , $z = z_{N-1}$, implying that det(A) ≠ 0 otherwise.

A couple of algorithms to calculate FD weights (continued)

Method 2: Taylor expand in an auxiliary variable:

Given linear operator L, equate as many Taylor coefficients as possible in ξ for

$$\sum_{k=1}^{N} w_k e^{z_k \xi} = L\, e^{z\xi}\Big|_{z=0}$$

This also results in a linear system for the weights w_k.

Example: $L = \dfrac{d^2}{dz^2}$, $\qquad L\, e^{z\xi}\Big|_{z=0} = \left\{ \quad \xi^2 \quad \right\}$

Example: $L\ f = \int_0^\infty f\ dz - h\sum_{k=0}^{\infty} f(k)$, $\qquad L\, e^{z\xi}\Big|_{z=0} = \left\{ \dfrac{h}{e^{h\xi}-1} - \dfrac{1}{\xi} \right\}$

Mathematica: $\mathrm{S} = \left\{ \qquad \right\} - \sum_{\mathrm{k}=1}^{\mathrm{N}} \mathrm{c[k]\, e^{-zk[[k]]\,\xi}};$

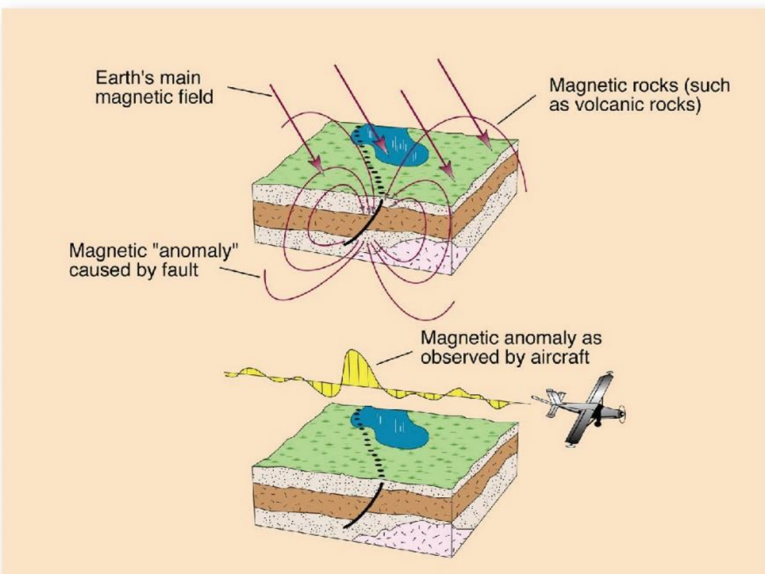
$$\mathrm{wk = Solve[LogicalExpand[Series[S,\{\xi,0,N-1\}]==0]]}$$

Note: The second example produces the weights in the Euler-Maclaurin stencils with no knowledge needed about its coefficients – or even that such an expansion exists.

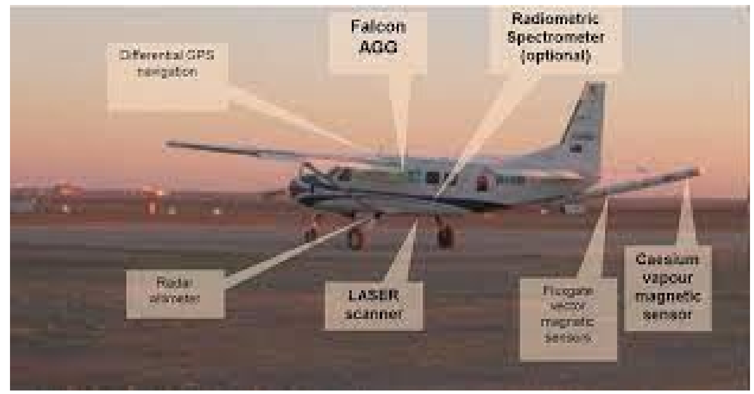
Current application: Mineral prospecting

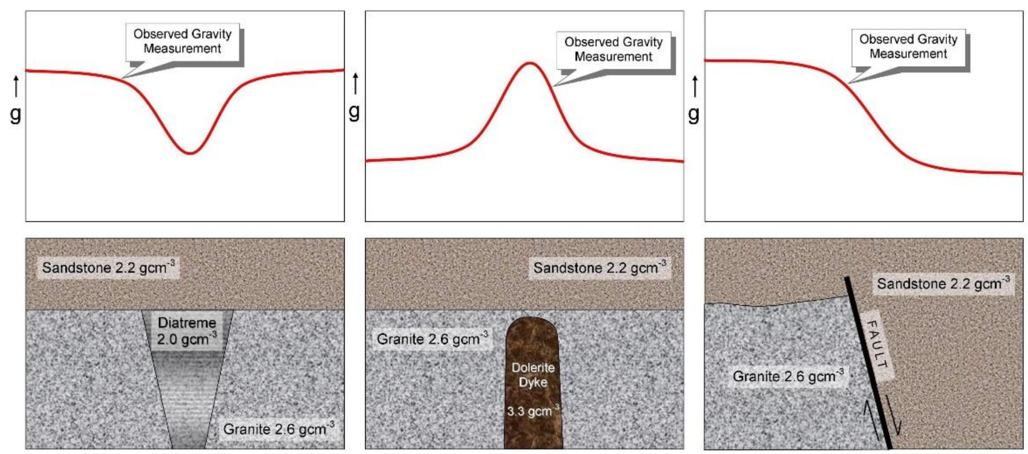
Collaboration with Jeff Thuston, *Intrepid Geophysics*
Data collected by airborne measurements of magnetic and gravity fields

Magnetic Surveys



Gravity Surveys



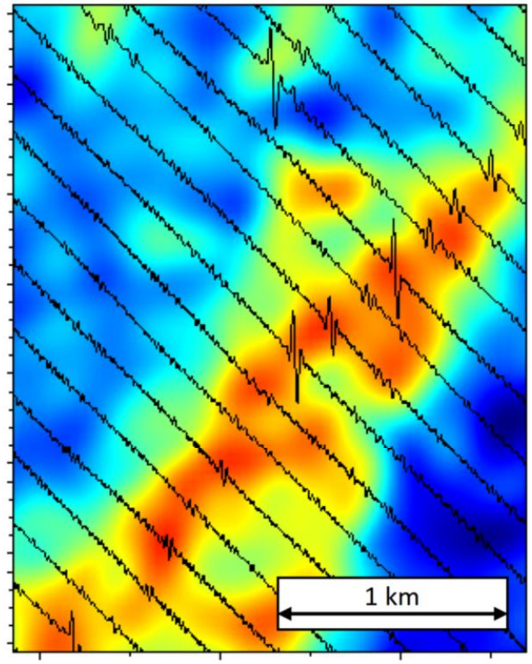


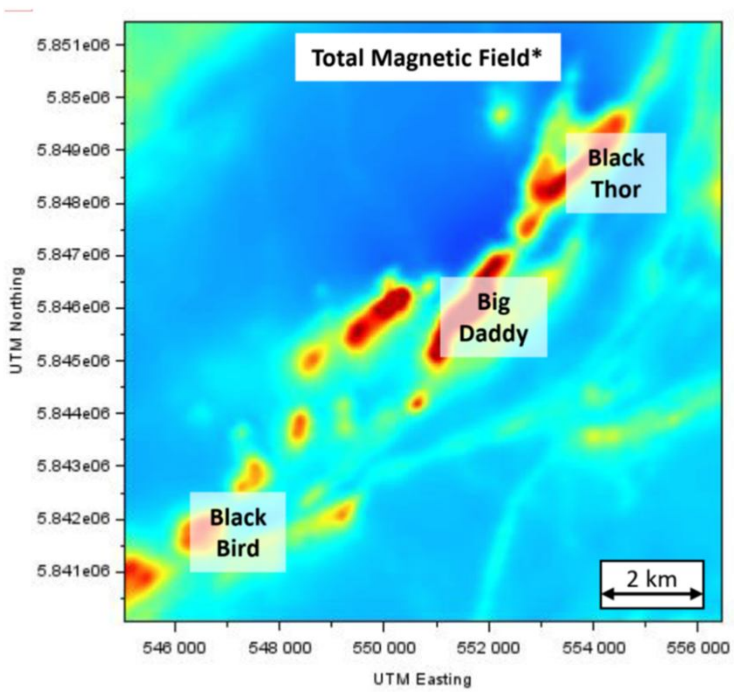
Planned chromium mining in *Ring of Fire*, Ontario, Canada

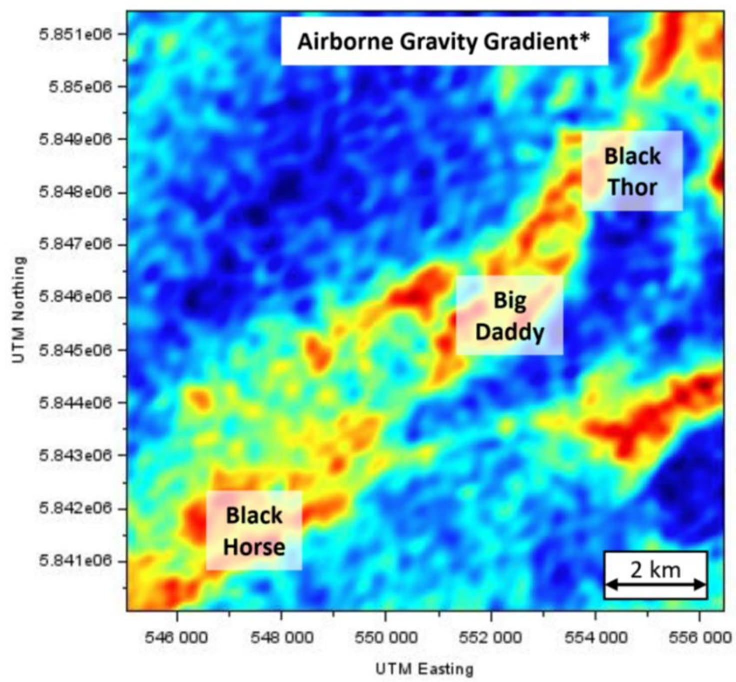
Data traces, followed by ‘state-ot-the-art’ postprocessing:

FFT based Hilbert transform; analytically continue downwards →

Recovered magnetic and gravity field anomalies ↓ ↘

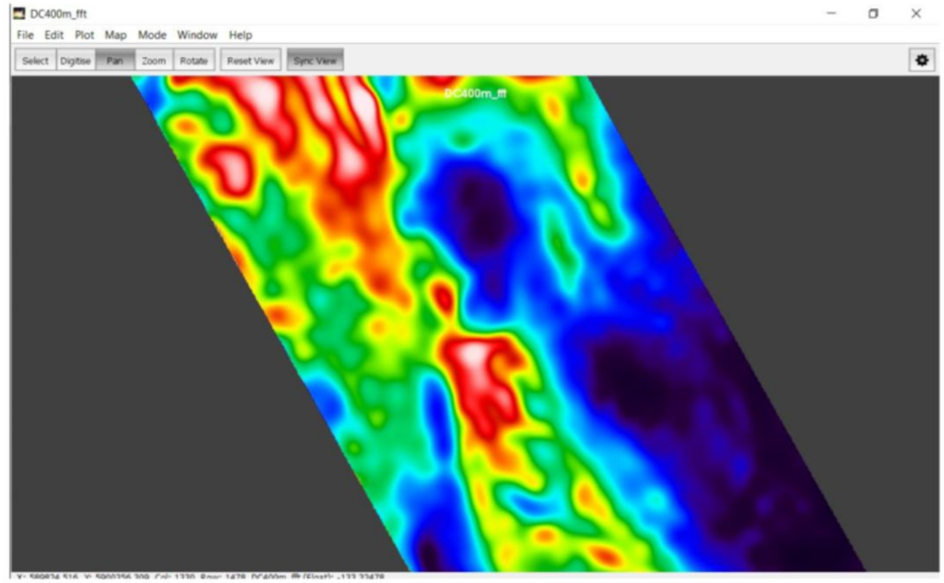




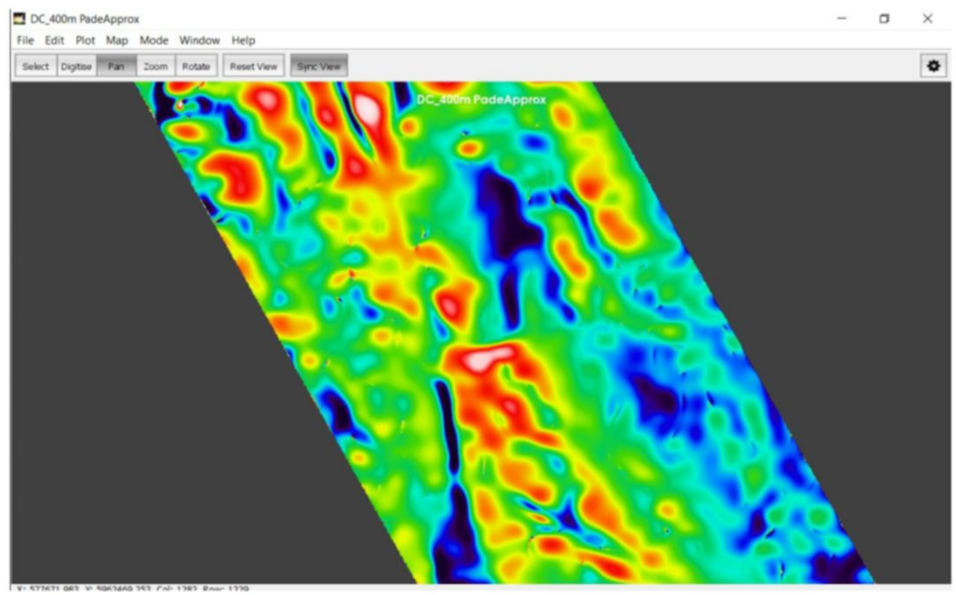


Comparison between postprocessing approaches:

‘Industry standard’
FFT + Hilbert transform continuation →

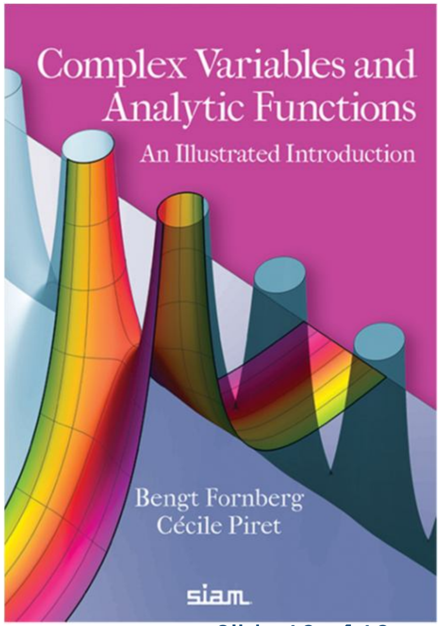


FFT + Hilbert transform providing data for complex plane FD formulas for up through the 5th derivative, followed by degrees {2,3} Padé continuation →



Some conclusions

- While ‘regular’ FD approximations have a long history, surprisingly little (if any) attention has previously been given to FD formulas specific to analytic (or harmonic) functions,
- Orders of accuracy in complex plane FD formulas increase similarly to total number of stencil points (rather than to the number of points in each spatial direction),
- The pseudospectral limit of increasing order FD approximations remains highly ‘local’, implying that high order stencils can be applied also near singularities,
- In the context of Euler-Maclaurin expansions, derivatives can be entirely replaced by function evaluations.
- Mathematical applications: Analytic continuation, PDEs in the complex plane
- Industrial application: Mineral prospecting



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