Numerical Methods in the Complex Plane

THE UNIVERSITY *of* EDINBURGH

Fred Dickinson
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Abstract

Two extensions of standard numerical methods to the complex plane are presented. This work is based on that from Prof. Bengt Fornberg (Fornberg, 2022) and James N. Lyness (Lyness, 1967).

The Complex-Step Derivative

Numerical approximations of function derivatives typically use finite difference formulae. The classical example is the forward difference

$$f'(x) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h),$$

but there are many variations of the theme, such as the backward difference or the more accurate $(\mathcal{O}(h^2))$ centred difference. An unfortunate feature these methods share is the subtraction operation in the numerator, leading to *subtractive cancellation* or *catastrophic cancellation* errors. To see this, let $\mathrm{fl}(x)$ be the floating-point representation of x. If f is smooth and h sufficiently small,

$$\mathrm{fl}[f(x+h)] = \mathrm{fl}[f(x)] \implies \mathrm{fl}[f(x+h)] - \mathrm{fl}[f(x)] = 0,$$

and hence the finite difference approximation yields zero.

The complex-step derivative takes finite differences into the complex plane. Analytic functions $f = u(z) + iv(z)$ of $z = x + iy$ satisfy the Cauchy-Riemann equations

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \quad \frac{\partial u}{\partial y} = \frac{\partial v}{\partial x},$$

and if f is real-valued with real arguments then $y = 0$ and $v(x) = 0$. With the standard definition of the derivative, it follows

$$f'(x) = \frac{\partial u}{\partial x} = \lim_{h \to 0} \frac{v(x+ih)}{h} = \lim_{h \to 0} \frac{\mathrm{Im}[f(x+ih)]}{h}.$$

Taking the discrete formulation of this expression gives you the *complex-step derivative.* By considering the Taylor expansion $f(x+ih)$, it can be shown this method is $\mathcal{O}(h^2)$ accurate (Squire and Trapp, 1998). Importantly, this approximation is *not* subject to subtractive cancellation.

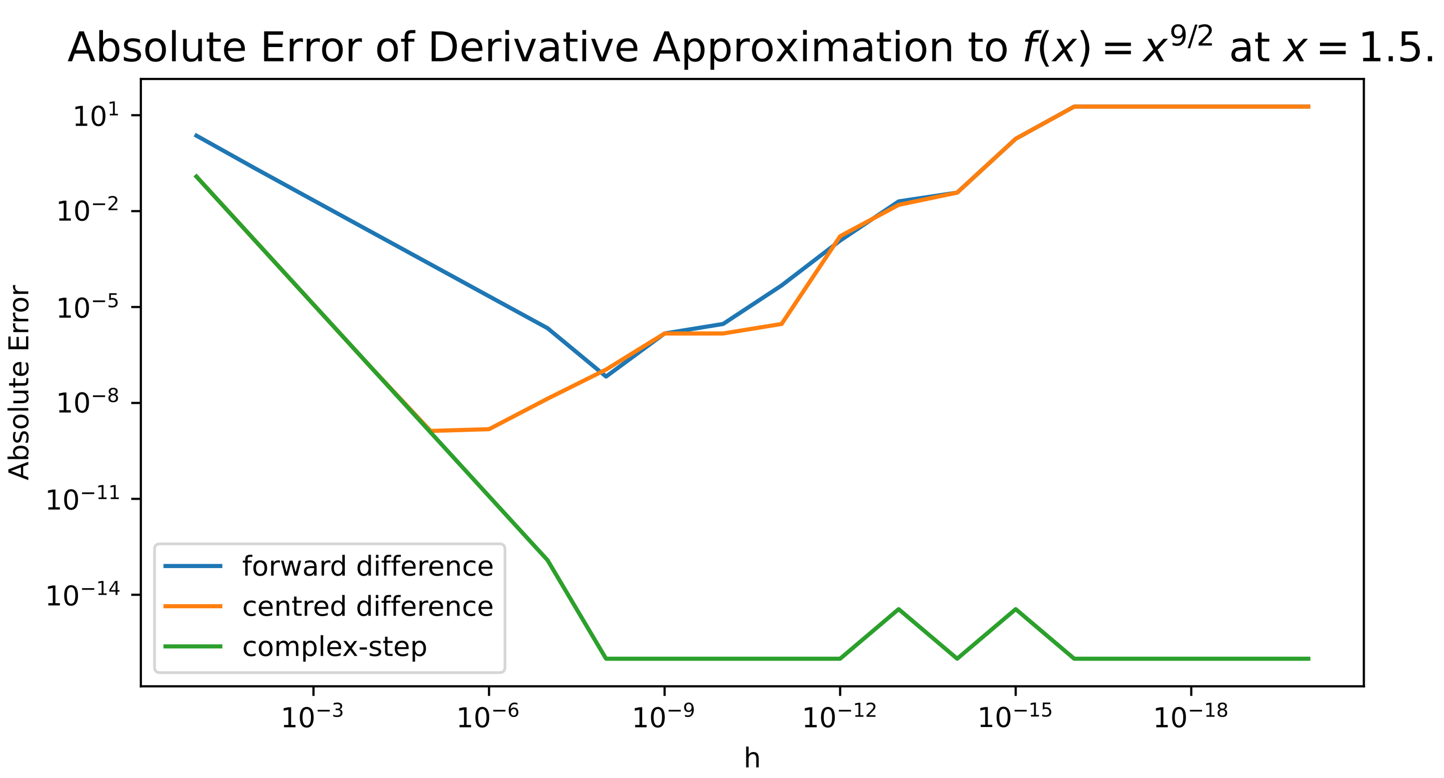

Figure 1: Finite difference approximations for $f(x) = x^{9/2}$ at $x = 1.5$ under log-log scaling. Convergence is as expected, with subtractive cancellation errors occurring from $h \approx 10^{-7}$. Data replicated from Squire and Trapp, 1998.

It must be noted that complex arithmetic operations take at least double the computational power than their real counterparts. This is the trade-off. Nonetheless, the method has become increasingly widespread, finding itself the subject of recent research such as the complex-step Newton method (Mitsotakis, 2025).

Variations of the Trapezoidal Rule

A common formulation of the trapezoidal rule evenly partitions intervals $[a, b]$ so that

$$\int_a^b f(x)\mathrm{d}x \approx h \left(\frac{f(x_0) + f(x_N)}{2} + \sum_{k=1}^{N-1} f(x_k) \right).$$

The nodes $x_0, x_1, \ldots, x_N$ lie on the real axis. Suppose these nodes are extended to the complex plane. One way to do this is to consider the endpoints as an $n \times n$ grid, or *'stencil'*, in $\mathbb{C}$.

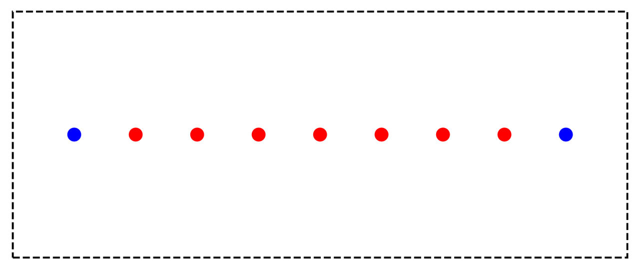

Figure 2: The standard trapezoidal rule has endpoints (blue) weighted with factor $1/2$, and the remaining points (red) weighted with factor 1.

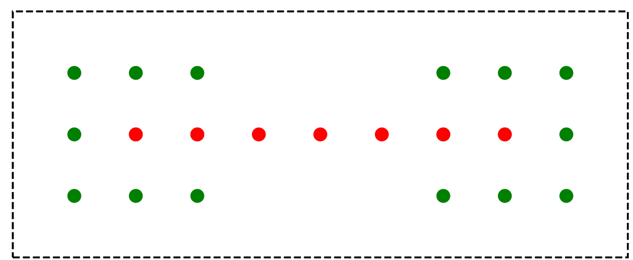

Figure 3: The trapezoidal rule with 3×3 'stencil' endpoints in $\mathbb{C}$. The stencil weights are green, and the line points (red) are again weighted with factor 1.

By introducing square $n \times n$ stencils at each endpoint, the accuracy of the trapezoidal rule increases to $\mathcal{O}(h^{n^2+1})$ (Fornberg, 2022). The example in Figure 3 is therefore of order $\mathcal{O}(h^{10})$; a significant improvement!

Determining the stencil weights is an exercise in coefficient matching. Consider a test function $f(z) = e^{z\xi}$ with the dummy variable $\xi : \mathrm{Re}(\xi) < 0$. For the sake of notation, suppose the integral to be approximated is on $[0, \infty)$. Fornberg shows the trapezoidal rule error is

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

where ζ is the famous Riemann-zeta function understood through analytic continuation. The correction stencil is designed to eliminate this error. Consider the stencil weights w_j at N given nodes z_j. Using the Taylor expansion of the exponential,

$$\sum_{j=1}^{N} w_j e^{z_j\xi} = \sum_{j=1}^{N} w_j \sum_{k=0}^{\infty} \frac{(z_j\xi)^k}{k!} = \sum_{k=0}^{\infty} \left(\frac{1}{k!} \sum_{j=1}^{N} w_j z_j^k \right) \xi^k.$$

Match the first $k = 0, 1, \ldots, K$ coefficients to form a linear system with a Vandermonde coefficient matrix. Then solve for the weights w_j. Simple implementations to do so in MatLab and Mathematica are provided (Fornberg, 2022).

References

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