The Complex-Step Method

Remember Complex/Imaginary Numbers?

Before we start, here's a (very) brief refresher on complex numbers

- $i = \sqrt{-1}$.
- A general complex number can be written as $z = x + iy$, where $x, y \in \mathbb{R}$.
- A complex number can be thought of as a point in the plane.

Like Finite-Differences, the Complex-Step Method Starts With Taylor Series

If $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is a function of real variables, and it is complex differentiable — which implies the function is complex analytic — on the domain of interest, then

Here is a Summary of the Complex-Step Approximation

Definition: Complex-Step Approximation [ST98]

The complex-step approximation of the partial derivative $\partial f / \partial x_j$ of the function $f : \mathbb{R}^n \to \mathbb{R}$ is given by

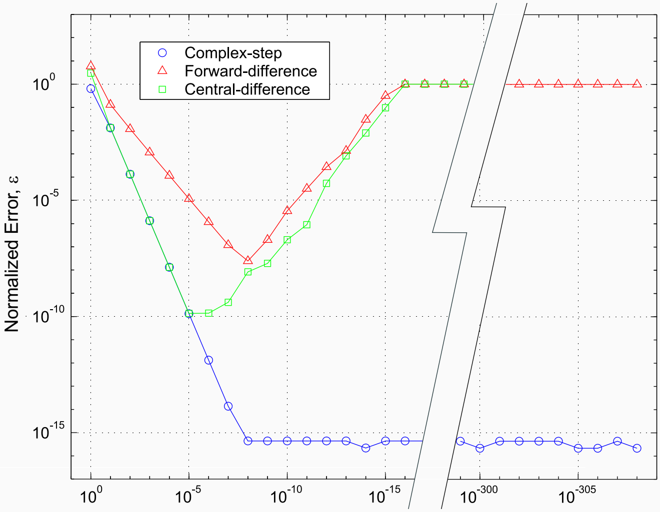
$$\frac{\Im[f(x + ihe_j)]}{h} = \frac{\partial f}{\partial x_j} + \underbrace{L_{\mathrm{CS}} h^2}_{\text{error}}$$

where $h > 0$ is the step size, e_j is the j^{th} Cartesian basis vector, and L_{CS} is a constant that does not depend on h.

The Complex-Step Approximation is Quite Remarkable

- The complex-step formula does not involve differences of function values;
- therefore, there is no subtractive cancellation due to round-off;
- therefore, we can make h as small as we want and make the error disappear!

The Complex-Step Approximation is Quite Remarkable (cont.)



Relative error in the derivative vs. decreasing step size

Pros & Cons of the Complex-Step Approximation

- ✓ easy to implement
- ✓ can be applied to almost any "black-box" software that accepts complex variables
- ✓ many open-source codes can be easily adapted to use complex-step.
- ✗ computational cost still scales with the # of design variables

References

William Squire and George Trapp, *Using complex variables to estimate derivatives of real functions*, SIAM Review **40** (1998), no. 1, 110–112.