Automatic Differentiation Using Complex and Hypercomplex Variables

Introduction to the Complex Taylor Series Expansion (CTSE) method for first order sensitivities

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Complex Taylor Series Expansion (CTSE)

- Complex variables can be used to compute accurate first order sensitivities. The derivation starts from the classical Taylor series expansion shown below.

$$f(x+h) \approx f(x) + \frac{df}{dx}h + \frac{1}{2}\frac{d^2f}{dx^2}h^2 + \frac{1}{3!}\frac{d^3f}{dx^3}h^3 + \frac{1}{4!}\frac{d^4f}{dx^4}h^4 + HOT$$

where h is the step, $\frac{d^nf}{dx^n}$ is the n'th derivative at (x), and HOT denotes the higher order terms.

If we replace real variable step h by an imaginary step ih, we obtain the following

$$f(x+ih) \approx f(x) + \frac{df}{dx}(x)(ih) + \frac{1}{2}\frac{d^2f}{dx^2}(x)(ih)^2 + \frac{1}{3!}\frac{d^3f}{dx^3}(x)(ih)^3 + \frac{1}{4!}\frac{d^4f}{dx^4}(x)(ih)^4 + HOT$$

$$= f(x) + \frac{df}{dx}(x)ih - \frac{1}{2}\frac{d^2f}{dx^2}(x)h^2 - \frac{1}{3!}\frac{d^3f}{dx^3}(x)ih^3 + \frac{1}{4!}\frac{d^4f}{dx^4}(x)h^4 + HOT$$

Complex Taylor Series Expansion (CTSE)

- The end result, separated into real and imaginary terms, is

$$f(x+ih) \approx \left(f(x) - \frac{1}{2}\frac{d^2f}{dx^2}h^2\right) + i\left(\frac{df}{dx}h - \frac{1}{3!}\frac{d^3f}{dx^3}ih^3\right) + HOT$$

The real result is

$$\mathrm{Re}(f(x+ih)) = f(x) + -\frac{1}{2}\frac{d^2f}{dx^2}h^2 + HOT$$

The imaginary result is

$$\mathrm{Im}(f(x+ih)) = \frac{df}{dx}h - \frac{1}{3!}\frac{d^3f}{dx^3}ih^3 + HOT$$

For sufficiently small h

$$f \approx \mathrm{Im}\left(f(x+ih)\right)$$

Real part unchanged.

$$\frac{df}{dx} \approx \frac{\mathrm{Im}(f(x+ih))}{h}$$

Imaginary part contains the first derivative.

Complex Taylor Series Expansion (CTSE)

- Summary, the first order derivative can be approximated as

For sufficiently small h

$$f \approx \mathrm{Re}\big(f(x + ih)\big)$$

$$\frac{df}{dx} \approx \frac{\mathrm{Im}(f(x + ih))}{h}$$

Note 1: that the derivative can be computed without any subtraction of terms, hence h can be made sufficiently small such that the terms of $O(h^2)$ can be reduced to below machine precision.

Note 2: the real part is also affected but again terms of order $O(h^2)$ can be reduced to below machine precision, hence, practically speaking, the real part is not affected.

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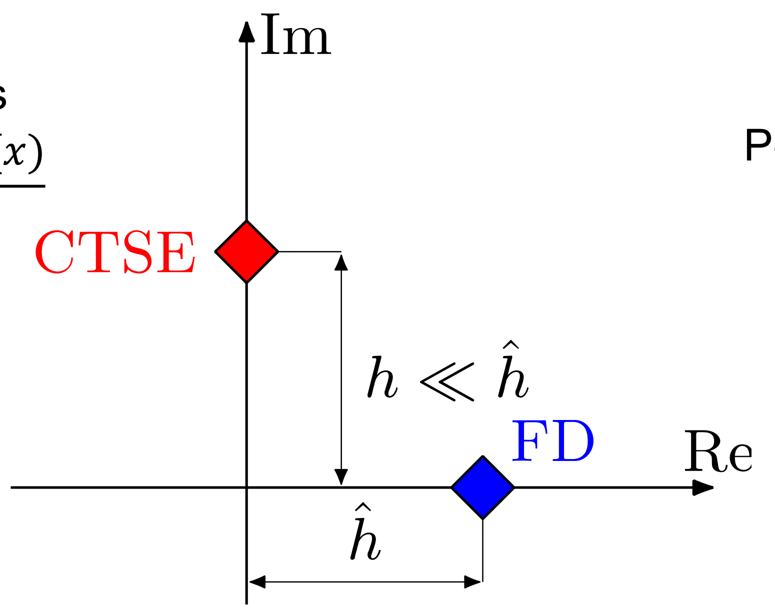
Analogy with the finite difference method

Finite Difference (FD)

Perturb along the real axis

$$\frac{df}{dx} \approx \frac{f(x+\hat{h}) - f(x)}{\hat{h}}$$

Subtraction errors occur when $h \to 0$



CTSE is performed analogously to FD

Complex Taylor Series Expansion (CTSE)

Perturb along the imaginary axis

$$\frac{df}{dx} \approx \frac{Im(f(x+ih))}{\hat{h}}$$

The step size can be made arbitrarily small with no concern about round-off error – **no subtraction error.**