Automatic Differentiation Using Complex and Hypercomplex Variables

Applying CTSE using the Cauchy-Reimann matrix format

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Cauchy-Reimann (CR) form

- CTSE can be employed without complex numbers using Cauchy-Reimann matrices of all real values. This is sometimes useful for numerical algorithms/software without a complex version, e.g., solvers for systems of linear equations.

Any complex number $a + bi$ can be rewritten in the matrix form $\begin{bmatrix} a & -b \\ b & a \end{bmatrix}$.

Thus, to differentiate a function using CTSE, one computes $f(x + ih) = f(\begin{bmatrix} x & -h \\ h & x \end{bmatrix})$ where h is again a small step size. Then

$$\frac{df}{dx} = \frac{f(\begin{bmatrix} x & -h \\ h & x \end{bmatrix})_{21}}{h}$$

Where the subscript 21 indicates the second row and first column of the resulting matrix.

Closed-form example: $f(x) = x^2$

- Compute the derivative of $f(x) = x^2$ using the CR form for complex numbers.

$$f(x) = x^2$$

$$f(x+ih) = \begin{bmatrix} x & -h \\ h & x \end{bmatrix}^2 = \begin{bmatrix} x^2 - h^2 & -2hx \\ 2hx & x^2 - h^2 \end{bmatrix}$$

$$\frac{df}{dx} = \frac{f\left(\begin{bmatrix} x & -h \\ h & x \end{bmatrix}\right)_{21}}{h} = \frac{1}{h}\begin{bmatrix} x^2 - h^2 & -2hx \\ 2hx & x^2 - h^2 \end{bmatrix}_{21} = 2x$$

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Closed-form example: $f(x) = x^3$

- Compute the derivative of $f(x) = x^3$ using the CR form for complex numbers.

$$f(x) = x^3$$

$$f(x+ih) = \begin{bmatrix} x & -h \\ h & x \end{bmatrix}^3 = \begin{bmatrix} x(x^2-h^2) - 2h^2x^2 & -h(x^2-h^2) - 2hx^2 \\ h(x^2-h^2) + 2hx^2 & x(x^2-h^2) - 2h^2x^2 \end{bmatrix}$$

$$\frac{df}{dx} = \lim_{h\to 0} \frac{f\left(\begin{bmatrix} x & -h \\ h & x \end{bmatrix}\right)_{21}}{h} =$$

$$\lim_{h\to 0} \frac{1}{h} \begin{bmatrix} x(x^2-h^2) - 2h^2x^2 & -h(x^2-h^2) - 2hx^2 \\ h(x^2-h^2) + 2hx^2 & x(x^2-h^2) - 2h^2x^2 \end{bmatrix}_{21} = x^2 + 2x^2 = 3x^2$$

CTSE is exact in the limit as $h \to 0$.

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Closed-form example: $f(x) = e^x$

- Compute the derivative of $f(x) = e^x$ using the CR form for complex numbers.

$$f(x) = e^x$$

$$f(x + ih) = expM\left(\begin{bmatrix} x & -h \\ h & x \end{bmatrix}\right) = \begin{bmatrix} e^x\cos(h) & -e^x\sin(h) \\ e^x\sin(h) & e^x\cos(h) \end{bmatrix}$$

$$\frac{df}{dx} = \lim_{h\to 0} \frac{f\left(\begin{bmatrix} x & -h \\ h & x \end{bmatrix}\right)_{21}}{h} =$$

$$\lim_{h\to 0} \frac{1}{h} \begin{bmatrix} e^x\cos(h) & -e^x\sin(h) \\ e^x\sin(h) & e^x\cos(h) \end{bmatrix}_{21} = e^x \frac{\sin(h)}{h} = e^x$$

CTSE is exact in the limit as $h \to 0$.

Note, **functions of matrices** must be used for the exponential operator NOT the standard exponential function.

Closed-form example: $f(x) = \sin(x)$

- Compute the derivative of $f(x) = \sin(x)$ using the CR form for complex numbers.

$$f(x) = \sin(x)$$

$$f(x + ih) = cosM(\begin{bmatrix} x & -h \\ h & x \end{bmatrix}) = \begin{bmatrix} \sin(x)\cosh(h) & -\cos(x)\sinh(h) \\ \cos(x)\sinh(h) & \sin(x)\cosh(h) \end{bmatrix}$$

$$\frac{df}{dx} = \lim_{h\to 0} \frac{f(\begin{bmatrix} x & -h \\ h & x \end{bmatrix})_{21}}{h} =$$

$$\lim_{h\to 0} \frac{1}{h} \begin{bmatrix} \sin(x)\cosh(h) & -\cos(x)\sinh(h) \\ \cos(x)\sinh(h) & \sin(x)\cosh(h) \end{bmatrix}_{21} = \cos(x)\frac{\sinh(h)}{h} = \cos(x)$$

CTSE is exact in the limit as $h \to 0$.

Note, **functions of matrices** must be used for the sine operator NOT the standard sine function.

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Closed-form example: $f(x) = \cos(x)$

- Compute the derivative of $f(x) = \cos(x)$ using the CR form for complex numbers.

$$f(x) = \cos(x)$$

$$f(x+ih) = cosM(\begin{bmatrix} x & -h \\ h & x \end{bmatrix}) = \begin{bmatrix} \cos(x)\cosh(h) & \sin(x)\sinh(h) \\ -\sin(x)\sinh(h) & \cos(x)\cosh(h) \end{bmatrix}$$

$$\frac{df}{dx} = \lim_{h\to 0} \frac{f(\begin{bmatrix} x & -h \\ h & x \end{bmatrix})_{21}}{h} =$$

$$\lim_{h\to 0} \frac{1}{h} \begin{bmatrix} \cos(x)\cosh(h) & \sin(x)\sinh(h) \\ -\sin(x)\sinh(h) & \cos(x)\cosh(h) \end{bmatrix}_{21} = -\sin(x)\frac{\sinh(h)}{h} = -\sin(x)$$

CTSE is exact in the limit as $h \to 0$.

Note, **functions of matrices** must be used for the cosine operator NOT the standard cosine function.

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Functions of matrices

- Functions of matrices[1] are not the same as the standard functions. For example,

$$Exp\begin{bmatrix} a & 0 \\ c & d \end{bmatrix} = \begin{bmatrix} e^a & 0 \\ \frac{c(e^a - e^d)}{a-d} & e^d \end{bmatrix}$$

$$Sin\begin{bmatrix} a & 0 \\ c & d \end{bmatrix} = \begin{bmatrix} \sin(a) & 0 \\ \frac{c(\sin(a) - \sin(d))}{a-d} & \sin(d) \end{bmatrix}$$

- Hence to use the CR form, one must have a language with good support of functions of matrices.

[1]Higham, Nicholas J. Functions of matrices: theory and computation. Society for Industrial and Applied Mathematics, 2008.

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Functions of matrices

- Note, some matrix functions loose accuracy for small h when using the complex variable CR form. Alternative: use the dual form of the CR matrix.

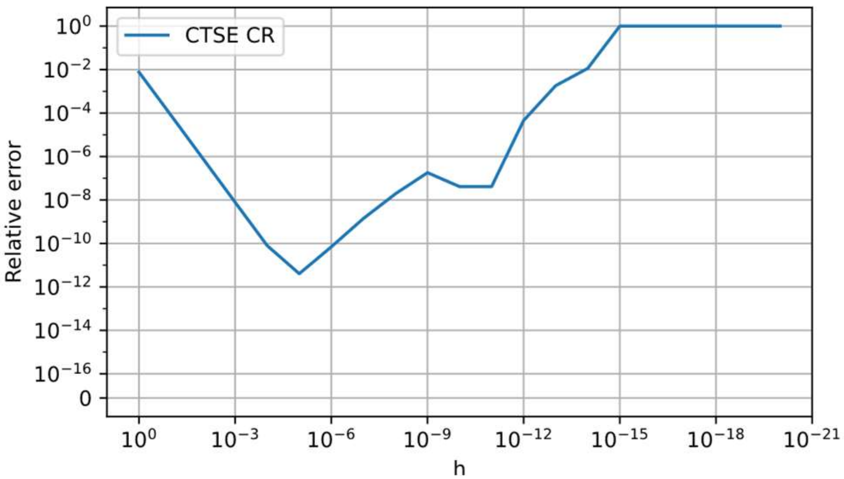
Complex form: $\begin{bmatrix} x & -h \\ h & x \end{bmatrix}$, h small

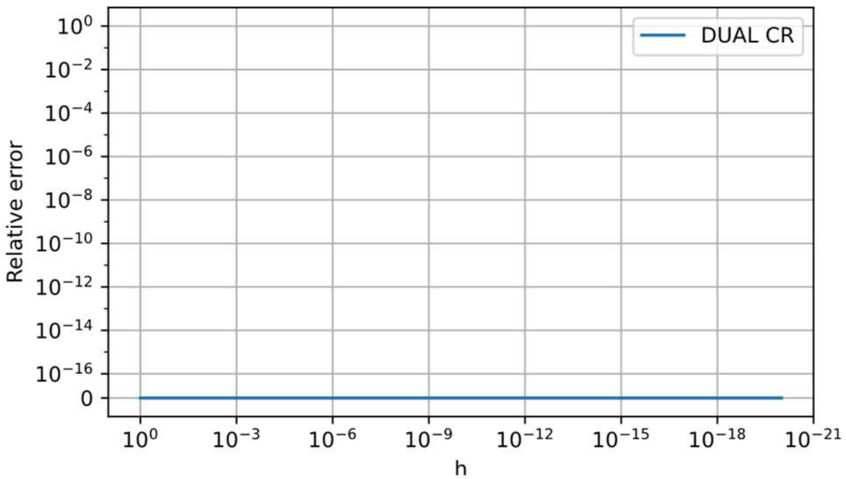
$$\frac{df}{dx} \approx \frac{sqrtM\left(\begin{bmatrix} x & -h \\ h & x \end{bmatrix}\right)_{21}}{h}$$

$$f(x) = \sqrt{x}$$

Dual form: $\begin{bmatrix} x & 0 \\ h & x \end{bmatrix}$, h arbitrary

$$\frac{df}{dx} = \frac{sqrtM\left(\begin{bmatrix} x & 0 \\ h & x \end{bmatrix}\right)_{21}}{h}$$





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