

Automatic Differentiation Using Complex and Hypercomplex Variables

Using dual numbers for first order sensitivities of complex functions

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Complex Functions

- Dual numbers can be used to compute first order derivatives of complex functions by perturbing the real portion, e.g., $f(x + \epsilon, y)$ then $\frac{df}{dz} = Im_{\epsilon}(f(x + \epsilon, y))$ where Im_{ϵ} means to extract the *dual* imaginary part (not the complex). Note, there will now be 2 different imaginary parts: i and ϵ . These two imaginary axes do not interact, that is $i * \epsilon$ does not simplify to -1 or 0 .

Example:

$$f(z) = z = x + iy$$

Perturb the real variable, i.e., $x = x + \epsilon$

$$f(x + \epsilon, iy) = (x + \epsilon) + iy$$

$$\frac{df}{dx} = Im_{\epsilon}(f(x + \epsilon)) = Im_{\epsilon}((x + \epsilon) + iy) = 1$$

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

$$f(z) = z^2 = (x + iy)^2 = x^2 + 2ixy - y^2$$

Analytical result

$$\frac{df}{dz} = 2x + 2iy = 2(x + iy) = 2z$$

Dual number approach

$$\begin{aligned} f(z + \epsilon) &= (x + \epsilon + iy)^2 = x^2 - y^2 + 2iy + 2(x + iy)\epsilon + \cancel{\epsilon^2} \\ &= (x^2 - y^2 + 2iy) + 2(x + iy)\epsilon \\ &= z^2 + 2z\epsilon \\ &= z + \frac{dz}{dz}\epsilon \end{aligned}$$

$$\frac{df}{dz} = \text{Im}_\epsilon(f(x + \epsilon), y) = \text{Im}_\epsilon((x + \epsilon, y)^2) = 2z$$

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

$$f(z) = z^3 = (x + iy)^3 = x^3 - 3xy^2 + i(3x^2y - y^3)$$

Analytical result

$$\frac{df}{dz} = 3x^2 - 3y^2 + i6xy = 3z^2$$

Dual number approach

$$\begin{aligned} f(z + \epsilon) &= (x + \epsilon + iy)^3 = x^3 - 3xy^2 + \epsilon^3 + 3\epsilon^2 + 3x^2\epsilon + -3y^2\epsilon \\ &\quad + i(3y\epsilon^2 + 6xy\epsilon + 3x^2y - y^3) \\ &= x^3 - 3xy^2 + i(3x^2y - y^3) + (3x^2 - 3y^2 + i(6xy))\epsilon \end{aligned}$$

$$= z^3 + 3z^2\epsilon$$

$$= z + \frac{dz}{dz}\epsilon$$

$$\frac{df}{dz} = \text{Im}_\epsilon(f(x + \epsilon), y) = \text{Im}_\epsilon((x + \epsilon, y)^3) = 3z^2$$

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

$$f(z) = \sin(z) = \sin(x + iy) = \sin(x) \cosh(y) + i \cos(x) \sinh(y)$$

Analytical result

$$\frac{df}{dz} \cos(x) \cosh(y) - i \sin(x) \sinh(y) = \cos(z)$$

Dual number approach

$$\begin{aligned} f(z + \epsilon) &= \sin(x + \epsilon) \cosh(y) + i \cos(x + \epsilon) \sinh(y) = \\ &(\sin(x) + \cos(x)\epsilon) \cosh(y) + i (\cos(x) + \sin(x)\epsilon) \sinh(y) = \\ \sin(x) \cosh(y) + i \cos(x) \sinh(y) + (\cos(x) \cosh(y) + i \sin(x) \sinh(y))\epsilon &= \\ \sin(z) + \cos(z) \epsilon & \\ &= z + \frac{dz}{dz} \epsilon \end{aligned}$$

$$\frac{df}{dz} = \text{Im}_\epsilon(f(x + \epsilon, y)) = \text{Im}_\epsilon(\sin(x + \epsilon, y)) = \cos(z)$$

CR form for complex-dual variables

- The CR form can be used to take numerical derivatives of complex functions. This can be done using a combined CR form for complex and dual numbers.

The CR dual form of a real number (with $h = 1$) is $\begin{bmatrix} R & 0 \\ 1 & R \end{bmatrix}$. Now replace R with the complex term z to yield $\begin{bmatrix} Z & 0 \\ 1 & Z \end{bmatrix}$. Finally replace Z with its CR form $Z = \begin{bmatrix} x & -y \\ y & x \end{bmatrix}$ to yield the final result

$$[z + \epsilon] = f\left(\begin{bmatrix} \text{Re}(z) & -\text{Im}_i(z) & 0 & 0 \\ \text{Im}_i(z) & \text{Re}(z) & 0 & 0 \\ 1 & 0 & \text{Re}(z) & -\text{Im}_i(z) \\ 0 & 1 & \text{Im}_i(z) & \text{Re}(z) \end{bmatrix}\right) =$$

$$f\left(\begin{bmatrix} x & -y & 0 & 0 \\ y & x & 0 & 0 \\ 1 & 0 & x & -y \\ 0 & 1 & y & x \end{bmatrix}\right)$$

CR form for complex-dual variables

- The real portion of the derivative ($\frac{df}{dz}$) will be contained in the 31 location of the CR output and the imaginary portion of the derivative will be contained in the 41 location.

The resulting output matrix will be

$$[z + \epsilon] = \begin{bmatrix} \text{Re}(f(x, y)) & -\text{Im}_i(f(x, y)) & 0 & 0 \\ \text{Im}_i(f(x, y)) & \text{Re}(f(x, y)) & 0 & 0 \\ \text{Re}(df/dz) & -\text{Im}_i(df/dz) & \text{Re}(f(x, y)) & -\text{Im}_i(f(x, y)) \\ \text{Im}(df/dz) & \text{Re}(df/dz) & \text{Im}_i(f(x, y)) & \text{Re}(f(x, y)) \end{bmatrix}$$

Then

$$\frac{df}{dx} = [z + \epsilon]_{31} + i[z + \epsilon]_{41} = 1$$

CR form for complex-dual variables: Example

$$f(x, y) = z = x + iy$$

- $f(x, y) = z = x + iy$

$$[z + \epsilon] = f \left(\begin{bmatrix} x & -y & 0 & 0 \\ y & x & 0 & 0 \\ 1 & 0 & x & -y \\ 0 & 1 & y & x \end{bmatrix} \right) = \begin{bmatrix} x & -y & 0 & 0 \\ y & x & 0 & 0 \\ 1 & 0 & x & -y \\ 0 & 1 & y & x \end{bmatrix}$$

Then

$$\frac{df}{dx} = [z + \epsilon]_{31} + i[z + \epsilon]_{41} = 1$$

CR form for complex-dual variables: Example

$$f(x, y) = z^2$$

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$$[z + \epsilon] = \begin{bmatrix} x & -y & 0 & 0 \\ y & x & 0 & 0 \\ 1 & 0 & x & -y \\ 0 & 1 & y & x \end{bmatrix}^2 = \begin{bmatrix} x^2 - y^2 & -2xy & 0 & 0 \\ 2xy & x^2 - y^2 & 0 & 0 \\ 2x & -2y & x^2 - y^2 & -2xy \\ 2y & 2x & 2xy & x^2 - y^2 \end{bmatrix}$$

Then

$$\frac{df}{dx} = [z + \epsilon]_{31} + i[z + \epsilon]_{41} = 2x + i2y = 2z$$

CR form for complex-dual variables: Example

$$f(x, y) = z^3$$

- $f(x, y) = z^3$

$$[z + \epsilon] = \begin{bmatrix} x & -y & 0 & 0 \\ y & x & 0 & 0 \\ 1 & 0 & x & -y \\ 0 & 1 & y & x \end{bmatrix}^3$$

$$= \begin{bmatrix} -2xy^2 + x(x^2 - y^2) & -2x^2y - y(x^2 - y^2) & 0 & 0 \\ 2x^2y + y(x^2 - y^2) & -2xy^2 + x(x^2 - y^2) & 0 & 0 \\ 3x^2 - 3y^2 & -6xy & -2xy^2 + x(x^2 - y^2) & -2x^2y - y(x^2 - y^2) \\ 6xy & 3x^2 - 3y^2 & 2x^2y + y(x^2 - y^2) & -2xy^2 + x(x^2 - y^2) \end{bmatrix}$$

Then

$$\frac{df}{dx} = [z + \epsilon]_{31} + i[z + \epsilon]_{41} = 3x^2 - 3y^2 + i6xy = 3z^2$$

CR form for complex-dual variables: Example

$f(x, y) = \sin(z)$

- $f(x, y) = \sin(z)$

Where $\sin M$ denotes the matrix sine function

$$[z + \epsilon] = \sin M \begin{bmatrix} x & -y & 0 & 0 \\ y & x & 0 & 0 \\ 1 & 0 & x & -y \\ 0 & 1 & y & x \end{bmatrix} =$$

$$\begin{bmatrix} \sin(x) \cosh(y) & -\cos(x) \sinh(y) & 0 & 0 \\ \cos(x) \sinh(y) & \sin(x) \cosh(y) & 0 & 0 \\ \cos(x) \cosh(y) & \sin(x) \sinh(y) & \sin(x) \cosh(y) & -\cos(x) \sinh(y) \\ -\sin(x) \sinh(y) & \cos(x) \cosh(y) & \cos(x) \sinh(y) & \sin(x) \cosh(y) \end{bmatrix}$$

Then

$$\frac{df}{dx} = [z + \epsilon]_{31} + i[z + \epsilon]_{41} = \cos(x) \cosh(y) - i \sin(x) \sinh(y) = \cos(x + iy) = \cos(z)$$