Automatic Differentiation Using Complex and Hypercomplex Variables

Approximating 2nd order derivatives using dual numbers

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Second Order Derivatives with Dual Numbers

- **Method**: Finite differences of dual numbers to obtain a second order derivative.
  - Evaluate first-order derivatives with dual numbers at two points: (x) and $(x + h_{FD})$:

$$\frac{df}{dx}(x) = Im(f(x + \epsilon)) \qquad \frac{df}{dx}(x + h_{FD}) = Im(f((x + h_{FD}) + \epsilon))$$

  - Apply Forward differences with the two evaluations to get the second derivative

$$\frac{d^2 f}{dx^2}(x) \approx \frac{\frac{df}{dx}(x + h_{FD}) - \frac{df}{dx}(x)}{h_{FD}} = \frac{Im(f((x + h_{FD}) + \varepsilon)) - Im(f(x + \varepsilon))}{h_{FD}}$$

  - Easily extended to Central Differences:

$$\frac{d^2 f}{dx^2}(x) \approx \frac{Im\Big(f((x + h_{FD}) + \varepsilon)\Big) - Im\Big(f((x - h_{FD}) + \varepsilon)\Big)}{2h_{FD}}$$

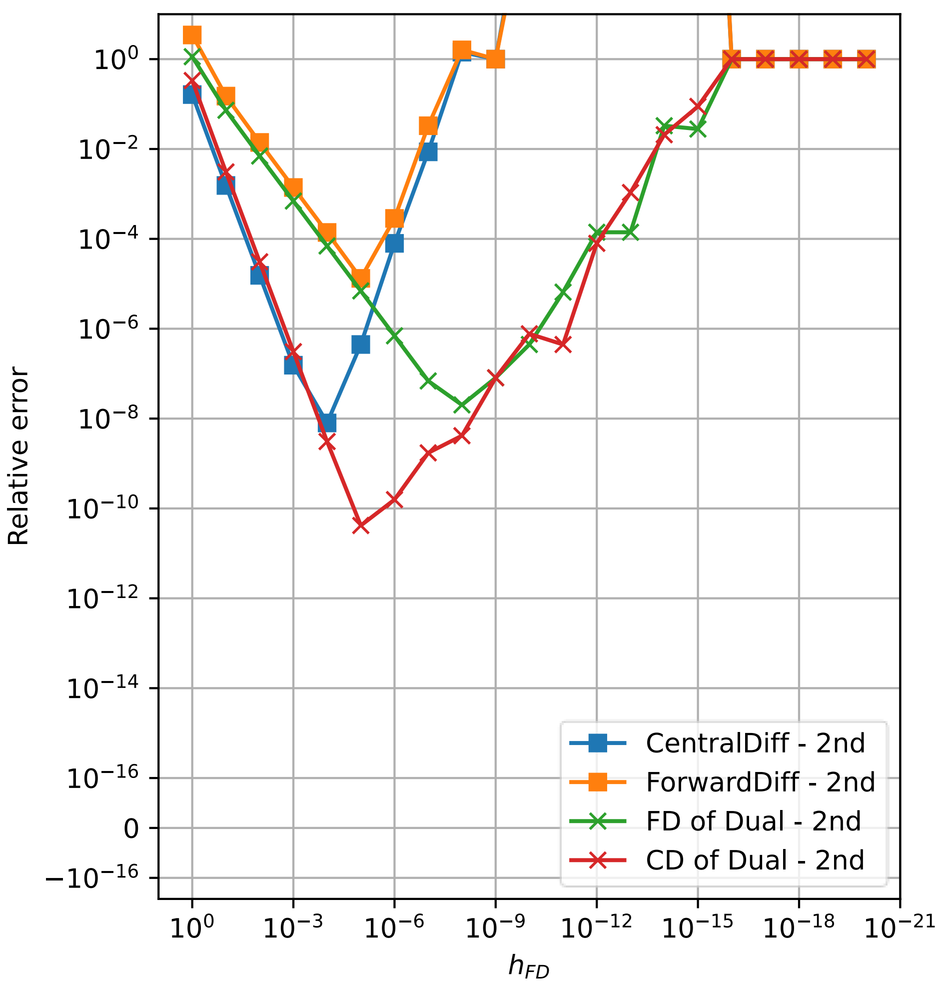
Second Order Derivatives with Dual Numbers

- Example: Closed form function: $f(x) = x^2 e^x$

Step size for dual first derivative was fixed at $h = 1$
Finite Differences for 2nd order derivatives:

ForwardDiff: $\frac{d^2 f}{dx^2}(x) \approx \frac{f(x+2h_{FD}) - 2f(x+h_{FD}) + f(x)}{h_{FD}^2}$

CentralDiff: $\frac{d^2 f}{dx^2}(x) \approx \frac{f(x+h_{FD}) - 2f(x) + f(x-h_{FD})}{h_{FD}^2}$



- Dual with finite differencing outperforms traditional finite difference methods.
- Second order derivatives suffers subtractive cancellation error.

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