Automatic Differentiation Using Complex and Hypercomplex Variables

Section 1: Approximating 2nd order derivatives with CTSE

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Second Order Derivatives with CTSE

- CTSE cannot be used to compute step-size independent 2nd order derivatives; however, it can be used to obtain an answer superior to that obtained from the standard finite difference method.

Method 1:
Finite differences of first-order derivatives obtained with CTSE.
- Forward differences
- Central differences

Requires *two complex function* evaluations.

Method 2:
Extract the second order derivative from the real coefficient of the CTSE evaluation
Requires *one complex and one real function* evaluations.

Both methods prone to subtractive cancellation error.

Second Order Derivatives with CTSE

- **Method 1**: Finite differences of CTSE to obtain a second order derivative.
  - Evaluate first-order derivatives with CTSE at two points: (x) and $(x + h_{FD})$:

$$\frac{df}{dx}(x) \approx \frac{Im\big(f(x+ih)\big)}{h}, \qquad \frac{df}{dx}(x + h_{FD}) \approx \frac{Im\Big(f\big((x + h_{FD}) + ih\big)\Big)}{h}$$

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

$$\frac{d^2 f}{dx^2}(x) \approx \frac{\frac{df}{dx}(x + h_{FD}) - \frac{df}{dx}(x)}{h_{FD}} = \frac{Im\Big(f\big((x + h_{FD}) + ih\big)\Big) - Im\big(f(x+ih)\big)}{h_{FD}\, h}$$

  - Easily extended to Central Differences:

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

Second Order Derivatives with CTSE

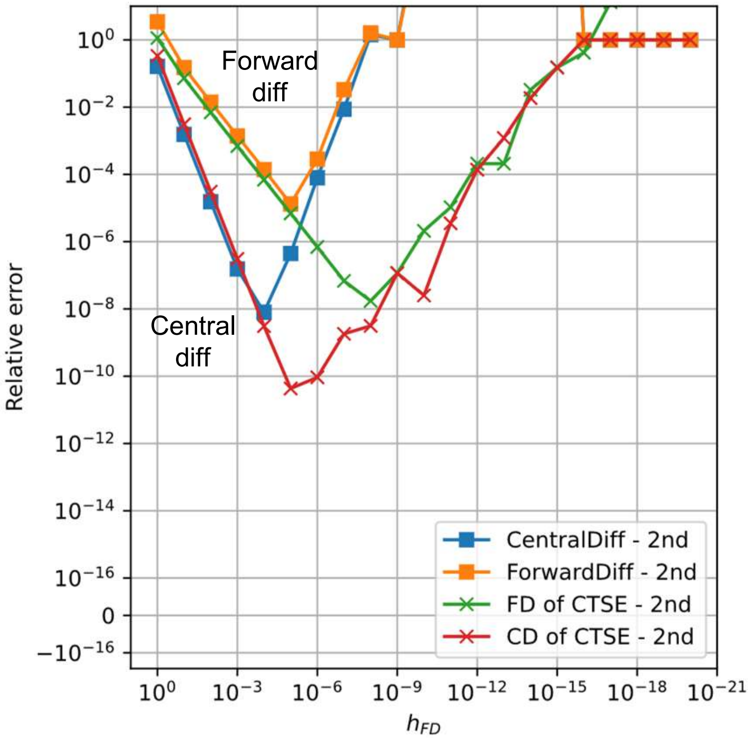
- Example **Method 1.** Closed form function: $f(x) = x^2 e^x$

Step size for CTSE first derivative was fixed at $h = 10^{-10}$.

Finite Differences for 2nd order derivatives:

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

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



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

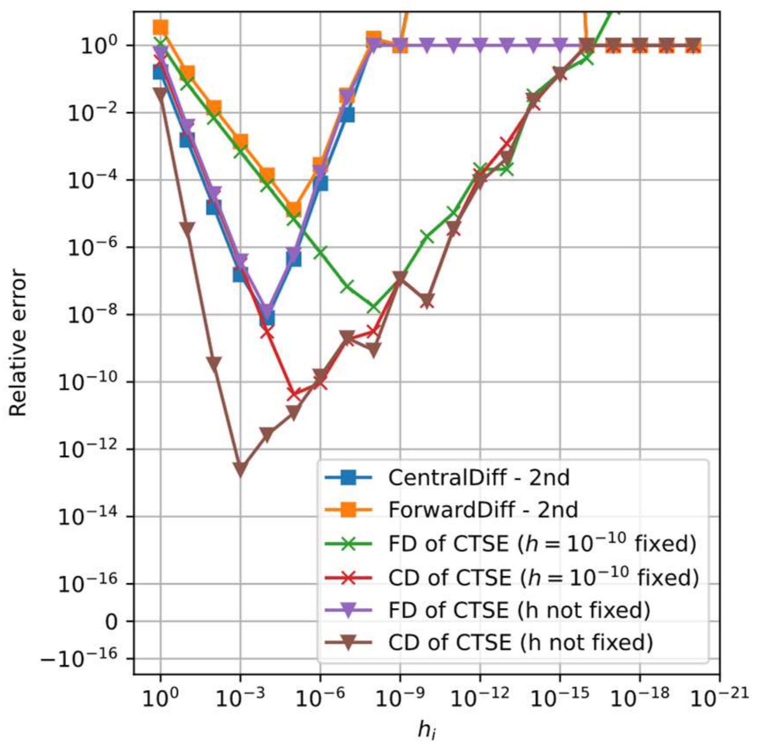
Second Order Derivatives with CTSE

- Best step-size for first-order with CTSE ≠ best step-size for second derivative with CTSE.

i.e. fixing the CTSE step size to $h = 10^{-1}$ is not best practice.

Lower errors can be achieved using different step-sizes:
For CTSE with CD → Best case $h_{FD} = h$
For CTSE with FD → Best case $h_{FD} = h^2$ *
*Can be particular to the function evaluated

- Selection of best step-size still very difficult.
- Subjected to subtractive cancellation error.



Second Order Derivatives with CTSE

- **Method 2:** Extract the second derivative from the real part of the CTSE evaluation.
- From the Complex Taylor Series Expansion:

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

The real part contains the second-order derivative:

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

Subtracting $f(x)$ from the real part leads to the second derivative

$$\frac{d^2f}{dx^2} \approx 2\frac{f(x) - Re\big(f(x+ih)\big)}{h^2} + HOT$$

In summary:

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

$$\frac{d^2f}{dx^2} \approx 2\frac{f(x) - Re\big(f(x+ih)\big)}{h^2}$$

Second Order Derivatives with CTSE

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

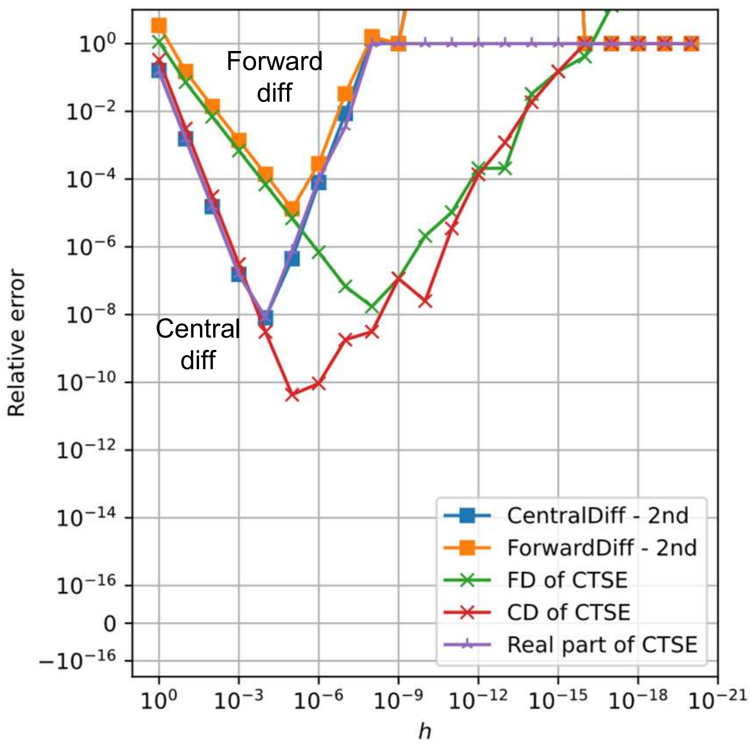
  Analytical solution:

$$\frac{d^2 f}{dx^2}(x) = (2 + 4x + x^2)e^x$$

  Approximation using CTSE

$$\frac{d^2 f}{dx^2}(x) \approx 2\,\frac{f(x) - \mathrm{Re}\big(f(x + ih)\big)}{h^2}$$

- Prone to subtractive cancellation error.
- Similar performance to CD with CTSE.



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Second Order Derivatives with CTSE

- Conclusion: Method 1 (apply FD to CTSE results) is slightly more accurate than Method 2 or classical CD.