Applying Dual numbers withing a numerical integration algorithm

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Application: Simpson's rule

- Let's study the behavior of using dual numbers to calculate the derivative of an integral using Simpson's rule.

$$I(a,b,c) = \int_a^b f(x,c)dx \approx \frac{b-a}{8}\left(f(a,c) + 3f\left(\frac{2a+b}{3}, c\right) + 3f\left(\frac{a+2b}{3}, c\right) + f(b,c)\right)$$

To calculate: $\frac{dI}{da} = Im(I(a+\epsilon, b, c)$, we replace a with $a+\epsilon$ within Simpson's rule.

$$I(a+\epsilon,b,c) = \int_a^b f(x,c)dx \approx \frac{b-(a+\epsilon)}{8}\left(f(a+\epsilon,c) + 3f\left(\frac{2(a+\epsilon)+b}{3}, c\right) + 3f\left(\frac{(a+\epsilon)+2b}{3}, c\right) + f(b,c)\right)$$

Then,

$$I = Re(I(a+\epsilon, b, c))$$

$$\frac{dI}{da} = Im(I(a+\epsilon, b, c))$$

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Application: Simpson's rule - $\frac{dI}{db}$

To calculate: $\frac{dI}{db} = Im(I(a, b+\epsilon, c)$, we replace b with $b+\epsilon$ within Simpson's rule.

$$I(a+\epsilon, b, c) = \int_a^b f(x,c)dx \approx \frac{(b+\epsilon)-a}{8}\left(f(a,c) + 3f\left(\frac{2a+(b+\epsilon)}{3}, c\right) + 3f\left(\frac{a+2(b+\epsilon)}{3}, c\right) + f(b+\epsilon, c)\right)$$

Then,

$$I = Re(I(a, b+\epsilon, c))$$

$$\frac{dI}{db} = Im(I(a, b+\epsilon, c))$$

Application: Simpson's rule - $\frac{dI}{dc}$

To calculate: $\frac{dI}{dc} = Im(I(a, b, c + \epsilon)$, we replace c with $c + \epsilon$ within Simpson's rule.

$$I(a + \epsilon, b, c) = \int_a^b f(x, c)dx \approx \frac{b - a}{8}\left(f(a, c + \epsilon) + 3f\left(\frac{2a + b}{3}, c + \epsilon\right) + 3f\left(\frac{a + 2b}{3}, c + \epsilon\right) + f(b, c + \epsilon)\right)$$

Then,

$$I = Re(I(a, b, c + \epsilon))$$

$$\frac{dI}{dc} = Im(I(a, b, c + \epsilon))$$

Application: Simpson's rule

- Example: $I(a,b,c) = \int_a^b xe^{-cx}dx$ with $a = 1, b = 2, c = 2$

	Exact	Dual Numbers	Relative Error
Integral	0.0786069	0.0785338	$9.3 * 10^{-4}$
dI/da	-0.135335	-0.134807	$3.9 * 10^{-3}$
dI/db	0.0366313	0.0363799	$6.9 * 10^{-3}$
dI/dc	-0.109643	-0.109557	$7.8 * 10^{-3}$

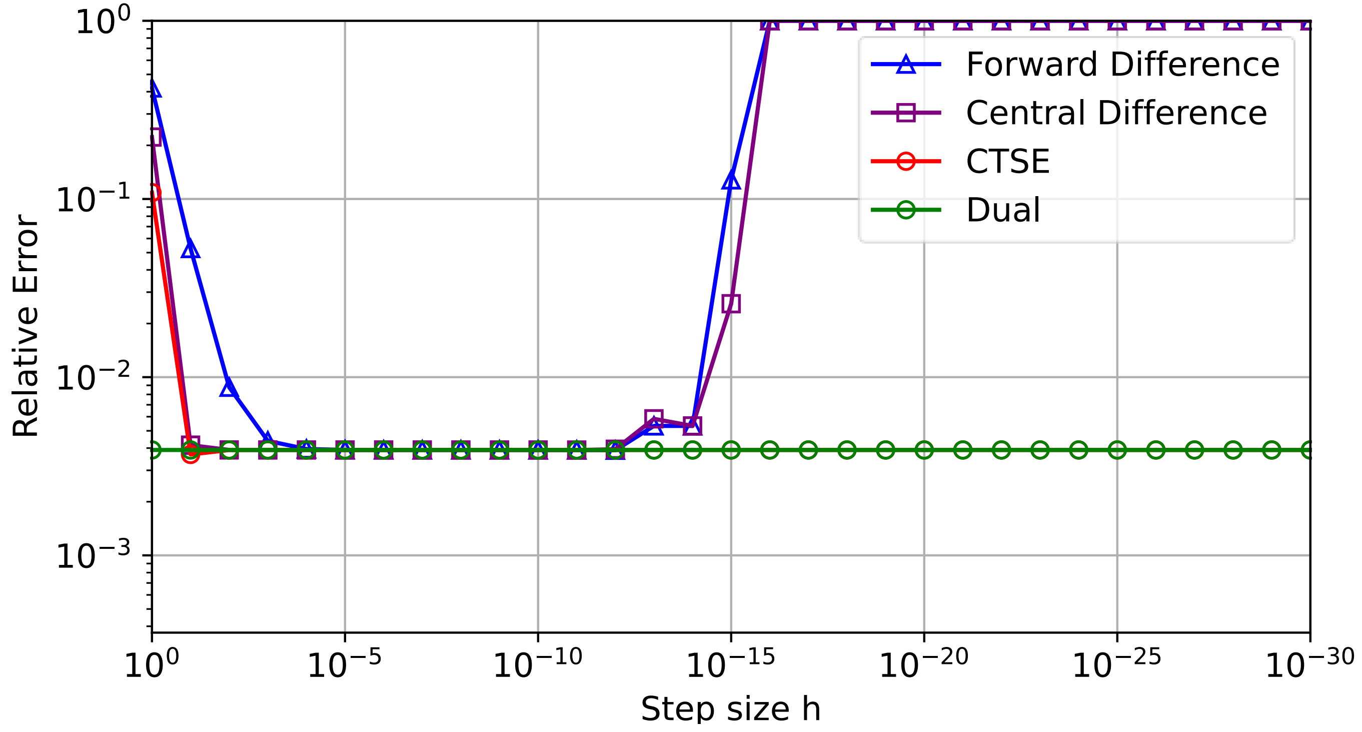
Note that the accuracy of the derivatives are ~one order less than the integral.
This behavior is often seen in applications.

The results are the same as when using CTSE.

Step size study – numerical integration

- A similar behavior will be seen for more complicated algorithms; however, dual numbers will not always provide machine precision accuracy– *the accuracy is dependent upon the algorithm in which it is deployed*.

$$\frac{\partial}{\partial a} I(a,b,c) = \frac{\partial}{\partial a}\left(\int_a^b x e^{-cx} dx\right) \text{ with } a = 1, b = 2, c = 2$$



$\frac{\partial}{\partial a} I(a,b,c)$ using Simpson's rule

Application: Gauss-Legendre quadrature

- Let's study the behavior of dual numbers to calculate the derivative the parameters of an integral using Gauss-Legendre quadrature.

$$I(a,b,c) = \int_a^b f(x,c) \approx \left(\frac{b\ -a}{2}\right)\sum_{i=1}^{n} w_i f\left(\frac{b\ -a}{2}\xi_i + \frac{b+a}{2}, c\right)$$

- Where w_i, ξ_i are weights and evaluation points, and n defines the number of integration points.
- As an example, consider $n = 3$ with the evaluation points $\xi = \left(-\sqrt{\frac{3}{5}}, 0, \sqrt{\frac{3}{5}}\right)$ with weights $w = \left(\frac{5}{9}, \frac{8}{9}, \frac{5}{9}\right)$ respectively.

Application: Gauss-Legendre quadrature

- To calculate: $dI/da \approx \frac{Im(I(a+\epsilon h,b,c)}{h}$, replace a with $a+\epsilon h$ within G-L quadrature and similarly for dI/db and dI/dc.

$$\frac{dI}{da} = \frac{Im(I(a+\epsilon h, b, c))}{h} \approx \frac{1}{h}\left(Im\left(\left(\frac{b\ -(a+\epsilon h)}{2}\right)\sum_{i=1}^{n} w_i f\left(\frac{b\ -(a+\epsilon h)}{2}\xi_i + \frac{b+(a+\epsilon h)}{2}, c\right)\right)\right)$$

$$\frac{dI}{db} = \frac{Im(I(a, b+\epsilon h, c))}{h} \approx \frac{1}{h}\left(Im\left(\left(\frac{(b+\epsilon h)-a}{2}\right)\sum_{i=1}^{n} w_i f\left(\frac{(b+\epsilon h)-a}{2}\xi_i + \frac{(b+\epsilon h)+a}{2}, c\right)\right)\right)$$

$$\frac{dI}{db} = \frac{Im(I(a, b, c+\epsilon h))}{h} \approx \frac{1}{h}\left(Im\left(\left(\frac{b\ -a}{2}\right)\sum_{i=1}^{n} w_i f\left(\frac{b\ -a}{2}\xi_i + \frac{b+a}{2}, c+\epsilon h\right)\right)\right)$$

Application: Gauss-Legendre quadrature

- Example: $I(a,b,c) = \int_a^b xe^{-cx} dx$ with $a = 1, b = 2, c = 2$.

	Exact	Gauss Quadrature	Relative Error
Integral	0.0786069	0.0786094	$3.17 * 10^{-5}$
dI/da	-0.135335	-0.135356	$1.55 * 10^{-4}$
dI/db	0.0366313	0.0366457	$3.93 * 10^{-4}$
dI/dc	-0.109643	-0.109642	$1.27 * 10^{-5}$

Dual results ($h = 1$ was used).

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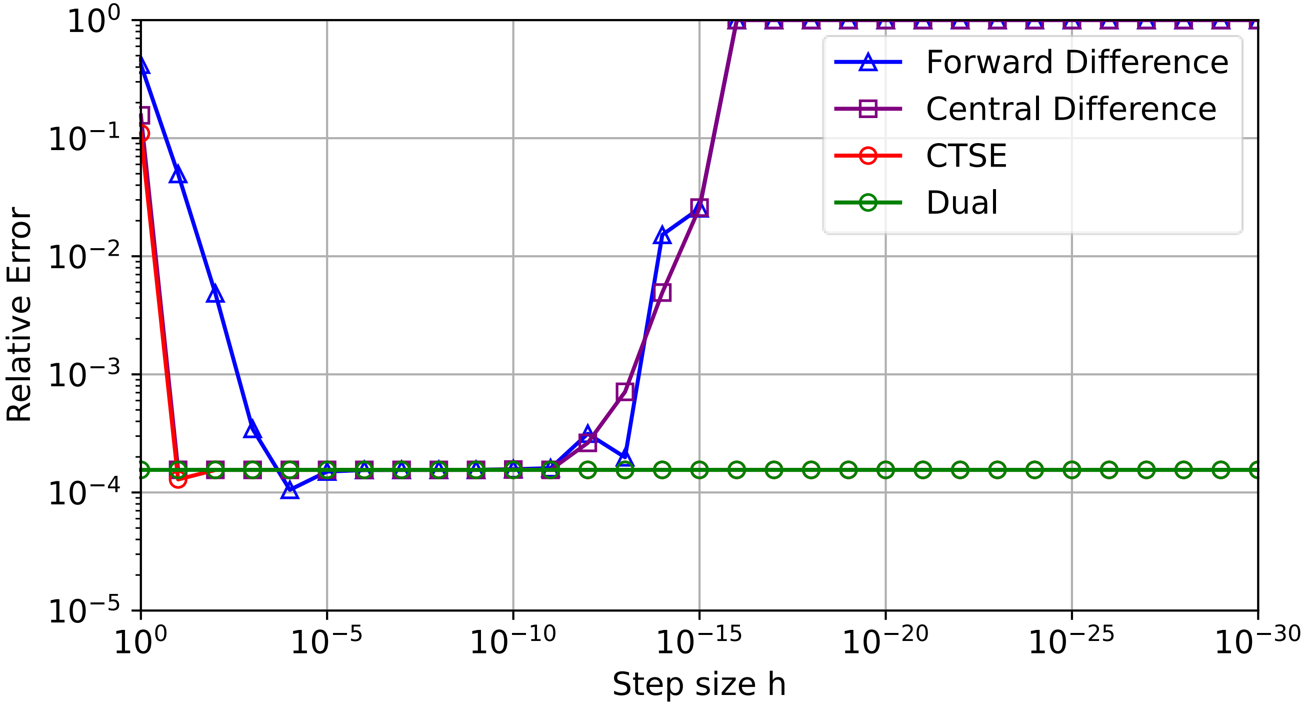
Application: Gauss-Legendre quadrature

- Observe the accuracy of the integral and its derivatives as a function of the step size for Dual, FD, and CD.

Relatve error using CTSE, FD, CD and dual numbers to calculate dI/dc.



- Dual results are step-size independent.
- FD and CD can also obtain the same accuracy but only for a window of h and the window is not known a priori.
- FD and CD “may” occasionally obtain a better result than dual numbers but this is a numerical artifact and rarely seen.