Automatic Differentiation Using Complex and Hypercomplex Variables

Applying CTSE within numerical integration algorithms

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Application: Simpson's rule

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

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: $\frac{dI}{da}\approx\frac{Im(I(a+ih,b,c)}{h}$, replace a with $a+ih$ within Simpson's rule.

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

Then,

$$I=Re(I(a+ih,b,c)$$

$$\frac{dI}{da}\approx\frac{Im(I(a+ih,b,c)}{h}$$

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Application: Simpson's rule, dI/db

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: $\frac{dI}{db} \approx \frac{Im(I(a,b+ih,c))}{h}$, replace b with $b+ih$ within Simpson's rule.

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

Then,

$$I = Re(I(a,b+ih,c))$$

$$\frac{dI}{db} \approx \frac{Im(I(a,b+ih,c))}{h}$$

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Application: Simpson's rule, dI/dc

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: $\frac{dI}{dc} \approx \frac{Im(I(a,b,c+ih))}{h}$, replace c with $c + ih$ within Simpson's rule.

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

Then,

$$I = Re(I(a,b,c+ih))$$

$$\frac{dI}{dc} \approx \frac{Im(I(a,b,c+ih))}{h}$$

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Application: Simpson's rule

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

	Exact	CTSE	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	$7.8 * 10^{-3}$

CTSE results ($h = 10^{-10}$ was used).

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

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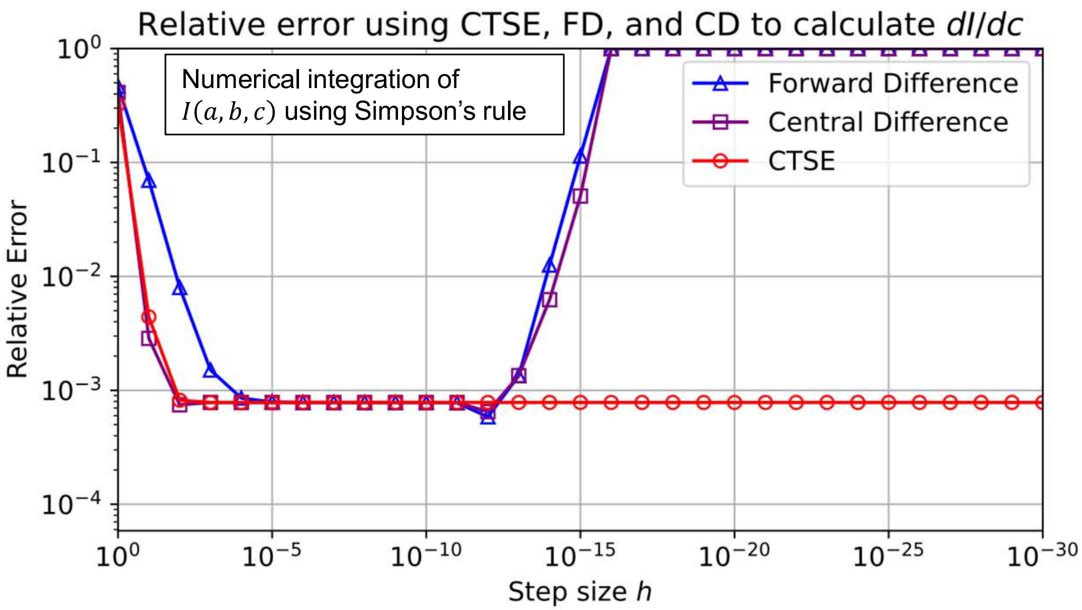
Application: Simpson's rule

- Observe the accuracy of the derivative dI/dc as a function of the step size for CTSE, FD, and CD.

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



- CTSE reaches an accurate result for $h < 10^{-3}$.
- FD and CD can also obtain the same accuracy but only for a window of h and the window is unknown a priori.

Application: Simpson's rule

- Compare the accuracy of dI/dc computed 2 ways: 1)CTSE applied directly to I, and 2) Integration of the analytical derivative. Both integrals computed using Simpson's rule.

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

$$\frac{dI_1}{dc} \approx \frac{1}{h} Im(I(a,b,c+ih))$$

$$\frac{dI_2}{dc} = \frac{d}{dc}\int_a^b xe^{-c}\ dx = \int_a^b \frac{d}{dc}(xe^{-cx})dx = \int_a^b(-x^2e^{-cx})dx$$

CTSE	Analytical derivative
$\frac{dI_1}{dc} \approx \frac{1}{h} Im(I(a,b,c+ih))$	$\frac{dI_2}{dc} = \int_a^b (-x^2e^{-cx})dx$
-0.109557440400866	-0.1096432776573800

To summarize, CTSE provides the most accurate numerical derivative possible (given sufficiently small step size) – the accuracy is only limited in this case by the accuracy of Simpson's rule.

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Application: Gauss-Legendre quadrature

- Let's study the behavior of CTSE 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.

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Application: Gauss-Legendre quadrature

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

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

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

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

Application: Gauss-Legendre quadrature

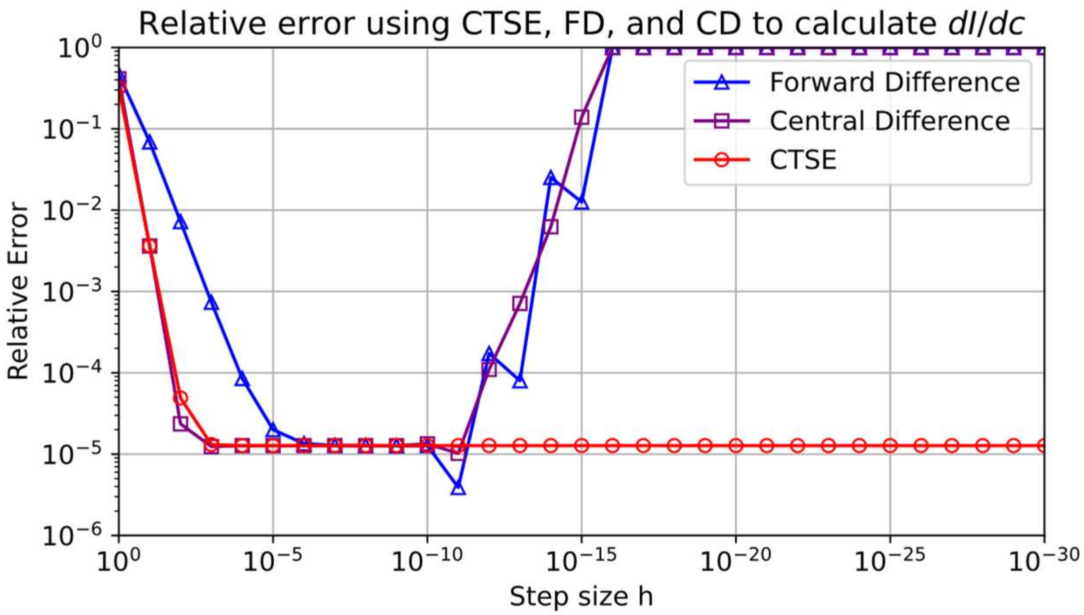
- Example: $I(a,b,c) = \int_a^b xe^{-cx}dx$ with $a = 1, b = 2, c = 2$.

	Exact	CTSE	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	$1.27 * 10^{-5}$

CTSE results ($h = 10^{-1}$ was used).

Application: Gauss-Legendre quadrature

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



- CTSE reaches an accurate result for $h < 10^{-3}$.
- 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 CTSE but this is a numerical artifact and rarely seen.