Automatic Differentiation Using Complex and Hypercomplex Variables

Section 3: Bidual numbers for first and second order sensitivities

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Bidual numbers - Overview

- Bidual numbers are an extension of dual numbers. They are useful for computing second order (either full or mixed) and first order sensitivities.
- Bidual numbers consist of 4 real coefficients (x_0, x_1, x_2, x_{12}) and three imaginary axes $(\epsilon_1, \epsilon_2, \epsilon_{12})$.
  - The imaginary axes are represented using the symbol ϵ.
  - The symbol ϵ is analogous to the imaginary symbol i from complex numbers; however, $\epsilon_i^2 = 0$; with $\epsilon \neq 0$. Also, $\epsilon_i \epsilon_j \neq 0$.

Example of a bidual number

$$x^* = x_0 + x_1\epsilon_1 + x_2\epsilon_2 + x_{12}\epsilon_{12}$$

Note, there is an analogous bicomplex number but bidual numbers are more robust and efficient.

$$x^* = x_0 + x_1 i_1 + x_2 i_2 + x_{12} i_{12}$$

Bidual numbers - Construction

- A Bidual number is constructed from two dual numbers.

$$B = D_1 + D_2\epsilon_2$$ Bidual

$$D_1 = x_0 + x_1\epsilon_1 \qquad D_2 = x_2 + x_3\epsilon_1$$ Dual

Expanded result

$$B = (x_0 + x_1\epsilon_1) + (x_2 + x_3\epsilon_1)\epsilon_2$$
$$= x_0 + x_1\epsilon_1 + x_2\epsilon_2 + x_3\epsilon_1\epsilon_2$$

Renumber $x_3 = x_{12}$ and $\epsilon_1\epsilon_2 = \epsilon_{12}$

$$B = x_0 + x_1\epsilon_1 + x_2\epsilon_2 + x_{12}\epsilon_{12}$$
$$= bidual(x_0, x_1, x_2, x_{12})$$ ← Short-hand notation:

Computing Derivatives using Bidual numbers – univariate example

- To use bidual numbers to compute derivatives for univariate functions, we perturb the variable of interest along 2 imaginary directions using step sizes h_1 and h_2. We do not perturb along ϵ_{12}. In general, we use use h_1 = h_2 =1.

General case

$$f(x^*) = f\big(bidual(x_0, h_1, h_2, 0)\big)$$

$$\frac{df}{dx} = \frac{1}{h_1} Im_1(f(x^*)) = \frac{1}{h_2} Im_2(f(x^*))$$

$$\frac{d^2 f}{dx^2} = \frac{1}{h_1 h_2} Im_{12}(f(x^*))$$

Recommended: $h_1 = h_2 = 1$

$$f(x^*) = f\big(bidual(x_0, \overset{x_1}{1}, \overset{x_2}{1}, \overset{x_{12}}{0})\big)$$

$$\frac{df}{dx} = Im_1(f(x^*)) = Im_2(f(x^*))$$

$$\frac{d^2 f}{dx^2} = Im_{12}(f(x^*))$$

Where Im_1 means extract the real coefficient of the $\epsilon_1$axes, Im_2 the ϵ_2 axes, andIm_{12} the ϵ_{12} axis.

Bidual number definition w MultiZ

- Bidual numbers can be specified using MultiZ then used as a traditional real number. MultiZ will handle the mathematical operations.

```
#Extracting the real and imaginary part of a multidual number.
#Note the input argument isindex or list of indices of the imaginary part
from multiZ.mdual import *
a = 5 + 3*eps(1) + 4*eps(2) + 7*eps([1,2])
a0 = a.real()
a1 = a.imag(1)
a2 = a.imag(2)
a12 = a.imag([1,2])
print(a0,a1,a2,a12)
#Outputs: 5.0, 3.0, 4.0, 7.0 the coefficents of the bidual number
```

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Bidual numbers – Addition/Subtraction

- Addition and subtraction of bidual numbers is accomplished part by part.

$$x^* = x_0 + x_1\epsilon_1 + x_2\epsilon_2 + x_{12}\epsilon_{12}$$
$$y^* = y_0 + y_1\epsilon_1 + y_2\epsilon_2 + y_{12}\epsilon_{12}$$

$$x^* \pm y^* = (x_0 \pm y_0) + (x_1 \pm y_1)\epsilon_1 + (x_2 \pm y_2)\epsilon_2 + (x_{12} \pm y_{12})\epsilon_{12}$$

Notation: an asterisk is used to indicate a hypercomplex number, e.g., “x^*”

Bidual numbers – Multiplication

- Multiplication of bidual numbers $a^* * b^*$ can be accomplished term by term and simplified using the properties $\epsilon_i^{\geq 2} = 0$ as shown. Consider the outer product of a^* and b^*:

$$\begin{array}{cc} & \begin{matrix} a_0 & a_1\epsilon_1 & a_2\epsilon_2 & a_{12}\epsilon_{12} \end{matrix} \\ \begin{matrix} b_0 \\ b_1\epsilon_1 \\ b_2\epsilon_2 \\ b_{12}\epsilon_{12} \end{matrix} & \begin{pmatrix} a_0 b_0 & a_0 b_1 \epsilon_1 & a_0 b_2 \epsilon_2 & a_0 b_{12} \epsilon_{12} \\ a_1 b_0 \epsilon_1 & a_1 b_1 \epsilon_1^2 & a_1 b_2 \epsilon_1 \epsilon_2 & a_1 b_{12} \epsilon_1 \epsilon_{12} \\ a_2 b_0 \epsilon_2 & a_2 b_1 \epsilon_1 \epsilon_2 & a_2 b_2 \epsilon_2^2 & a_2 b_{12} \epsilon_2 \epsilon_{12} \\ a_{12} b_0 \epsilon_{12} & a_{12} b_1 \epsilon_1 \epsilon_{12} & a_{12} b_2 \epsilon_2 \epsilon_{12} & a_{12} b_{12} \epsilon_{12}^2 \end{pmatrix} \end{array}$$

Terms in dark red are zero due to:

$$\epsilon_i^2 = 0$$

$$\epsilon_1 \epsilon_{12} = \epsilon_1 \epsilon_1 \epsilon_2 = \epsilon_1^2 \epsilon_2 = 0$$

$$\epsilon_2 \epsilon_{12} = \epsilon_1 \epsilon_2 = \epsilon_1^2 \epsilon_2^2 = 0$$

Bidual numbers – Multiplication

- After removing the zero terms we have:

$$x^* * y^* = \begin{pmatrix} x_0y_0 & x_0y_1\epsilon_1 & x_0y_2\epsilon_2 & x_0y_{12}\epsilon_{12} \\ x_1y_0\epsilon_1 & 0 & x_1y_2\epsilon_{12} & 0 \\ x_2y_0\epsilon_2 & x_2y_1\epsilon_{12} & 0 & 0 \\ x_{12}y_0\epsilon_{12} & 0 & 0 & 0 \end{pmatrix}$$

Gathering terms we have:

$$x^* * y^* = x_0y_0 + (x_0y_1 + x_1y_0)\epsilon_1 + (x_0y_2 + x_2y_0)\epsilon_2 + (x_0y_{12} + x_1y_2 + x_2y_1 + x_{12}y_0)\epsilon_{12}$$

Bidual numbers – Division

- Consider the division of 2 bidual numbers $\frac{x^*}{y^*}$. This result can be determined using the conjugate operation for ϵ_2 followed by a conjugate operation for ϵ_1. The end result is shown below. The derivation is presented in the reference for MultiZ. (See the CR section for an alternate derivation using matrices.)

$$\frac{x^*}{y^*} = \frac{x_0}{y_0} + \left(\frac{x_1}{y_0} - \frac{x_0 y_1}{y_0^2}\right)\epsilon_1 + \left(\frac{x_2}{y_0} - \frac{x_0 y_2}{y_0^2}\right)\epsilon_2 + \left(\frac{x_{12}y_0^3 - x_2 y_1 y_0^2 - y_2 y_0^2 + 2x_0 y_0 y_1 y_2 - x_0 y_0^2 y_{12}}{y_0^4}\right)\epsilon_{12}$$

A.M. Aguirre-Mesa, M.J. Garcia, and H.R. Millwater, "MultiZ: A library for computation of high order derivatives using multicomplex or multidual numbers," ACM Trans. Math. Softw. 46, 3, Article 23 (July 2020), 30 pages, https://doi.org/10.1145/3378538

Bidual numbers – Reciprocal

- The reciprocal of a bidual number is a subset of division.

$$\frac{1}{x^*} = \frac{1}{x_0} - \frac{x_1}{x_0^2}\epsilon_1 - \left(\frac{x_2}{x_0^2}\right)\epsilon_2 + \left(\frac{2x_0x_1x_2 - x_0^2x_{12}}{x_0^4}\right)\epsilon_{12}$$

Functions of Bidual numbers

- Functions of bidual numbers can be developed using the Taylor series expansion as shown below.

$$f(x^*) \approx f(x_0) + \sum_{k=1}^{n} \frac{f^{(k)}(x_0)}{k!}(x^* - x_0)^k$$

where for bidual numbers $n = 2$

$$f(x^*) \approx f(x_0) + f^{(k)}(x_0)(x^* - x_0) + \frac{1}{2} f^{(2)}(x_0)(x^* - x_0)^2$$

Functions of Bidual numbers

- Notice that the function f is only applied to the real coefficient x_0.

$$f(x^*) \approx f(x_0) + f^{(k)}(x_0)(x^* - x_0) + \frac{1}{2} f^{(2)}(x_0)(x^* - x_0)^2$$

$$(x^* - x_0) = bidual(0, x_1, x_2, x_{12})$$

and

$$(x^* - x_0)^2 = bidual(0, x_1, x_2, x_{12})^2 = bidual(0,0,0,2x_1x_2)$$

Apply the specific form of the Taylor series to each function.

Exponential of Bidual numbers

- The Taylor series for the exponential function can be written as

$$e^{x^*} \approx e^{x_0}[1 + \sum_{k=1}^{2} \frac{1}{k!}(x^* - x_0)^k] =$$

$$e^{x_0}\left[1 + (x^* - x_0) + \frac{1}{2}(x^* - x_0)^2\right] =$$

$$e^{x_0}\left[1 + bidual(0, x_1, x_2, x_{12}) + \frac{1}{2}bidual(0,0,0,2x_1x_2)\right] =$$

$$e^{x_0} + x_1 e^{x_0}\epsilon_1 + x_2 e^{x_0}\epsilon_2 + (x_1x_2 + x)e^{x_0}\epsilon_{12}$$

Note, if $x_1 = x_2 = 1\ and\ x_{12} = 0$

$$Exp(a_0, 1,1,0) = e^{x_0} + e^{x_0}\epsilon_1 + e^{x_0}\epsilon_2 + e^{x_0}\epsilon_{12}$$

Log of Bidual numbers

- The Taylor series for the natural log function can be written as

$$\log(x^*) \approx \log(x_0) + \sum_{k=1}^{2} \frac{(-1)^{k-1}}{k x_0^k} (x^* - x_0)^k] =$$

$$\log(x_0) + \frac{x - x_0}{x_0} - \frac{(x - x_0)^2}{2x_0^2} =$$

$$\log(x_0) + \frac{bidual(0, x_1, x_2, x_{12})}{x_0} - \frac{bidual(0,0,0,2x_1x_2)}{2x_0^2}$$

$$log(x_0) + \frac{x_1}{x_0}\epsilon_1 + \frac{x_2}{x_0}\epsilon_2 + \frac{(x_0 x_{12} - x_1 x_2)}{x_0^2}\epsilon_{12}$$

Note, if $x_1 = x_2 = 1 \; and \; x_{12} = 0$

$$\log(x_0, 1,1,0) = \log(x_0) + \frac{1}{x_0}\epsilon_1 + \frac{1}{x_0}\epsilon_2 - \frac{1}{x_0^2}\epsilon_2]$$

Sine of Bidual numbers

- The Taylor series for the sine function can be written as

$$\sin(x^*) \approx \sin(x_0) + \cos(x_0)(x^* - x_0) - \frac{1}{2}\sin(x_0)(x^* - x_0)^2 =$$

$$\sin(x_0) + \cos(x_0)\, bidual(0, x_1, x_2, x_{12}) - \frac{1}{2}\sin(x_0)\, bidual(0{,}0{,}0{,}2x_1x_2) =$$

$$sin(x_0) + a_1 cos(x_0)\epsilon_1 + a_2\, cos(x_0)\epsilon_2 + (a_{12}\, cos(x_0) - a_1a_2\, sin(x_0))\epsilon_{12}$$

Note, if $x_1 = x_2 = 1\ and\ x_{12} = 0$

$$\sin(x_0, 1{,}1{,}0) = sin(x_0) + cos(x_0)\epsilon_1 + cos(x_0)\epsilon_2 - sin(x_0)\epsilon_{12}$$

Cosine of Bidual numbers

- The Taylor series for the cosine function can be written as

$$\cos(x^*) \approx \cos(x_0) - \sin(x_0)(x^* - x_0) - \frac{1}{2}\cos(x_0)(x^* - x_0)^2 =$$

$$\cos(x_0) - \sin(x_0)\, bidual(0, x_1, x_2, x_{12}) - \frac{1}{2}\cos(x_0)\, bidual(0,0,0,2x_1x_2) =$$

$$cos(x_0) - x_1\, sin(x_0)\epsilon_1 - x_2\, sin(x_0)\epsilon_1 + (-x_{12}\, sin(x_0) - x_1\, x_2\, cos(x_0))\epsilon_{12}$$

Note, if $x_1 = x_2 = 1\ and\ x_{12} = 0$

$$\cos(x_0, 1,1,0) = cos(x_0) - sin(x_0)\epsilon_1 - sin(x_0)\epsilon_1 - cos(x_0)\epsilon_{12}$$

Bidual raised to a bidual number

- A bidual number raised to a bidual number can be evaluated in terms of the exponential and logarithmic functions

Use the formula $x^y = e^{yln(x)}$

This formula can be implemented with bidual numbers using the previously defined exponential and logarithmic functions.

$$a^{*\mathrm{b}^*} = e^{b^* ln(a^*)}$$

Bidual number a^* raised to a real number n

$$(a^*)^n = a_0^n + n a_0^{n-1} a_1 \epsilon_1 + n a_0^{n-1} a_1 \epsilon_2 + n a_0^{n-2}\left((n-1)a_1 a_2 + a_0 a_{12}\right) \epsilon_{12}$$

Real number r raised to a bidual number a^*

$$r^a = r^{a_0} + r^{a_0} \log(r) a_1\, \epsilon_1 + r^{a_0} \log(r) a_2\, \epsilon_2 + r^{a_0} \log(r)(\log(r)\, a_1 a_2 + a_{12})\ \epsilon_{12}$$

Derived functions of Bidual numbers

- Many functions can be derived in terms previously defined functions

$$\tan(a^*) = \frac{\sin(a^*)}{\cos(a^*)} =$$
$$\tan(a_0) + a_1 \sec(a_0)^2\, \epsilon_1 + a_2 \sec(a_0)^2\, \epsilon_2 + \sec(a_0)^2\, (a_{12} + 2a_1 a_2 \tan(a_0))\, \epsilon_{12}$$

Note: $\tan(bidual(x_0, 1,1,0)) = \tan(x_0) + \sec(x_0)^2\, \epsilon_1 + \sec(x_0)^2\, \epsilon_2 + 2\sec(x_0)^2 \tan(x_0)\, \epsilon_{12}$

$$\text{sqrt}(x^*) = (x^*)^{1/2} =$$
$$\sqrt{x_0} + \frac{x_1}{2\sqrt{x_0}}\epsilon_1 + \frac{x_2}{2\sqrt{x_0}}\epsilon_1 + \frac{-x_1 x_2 + 2x_{12}x_0}{4x_0^{3/2}}\epsilon_{12}$$

Note: $sqrt(bidual(x_0, 1,1,0)) = \sqrt{x_0} + \frac{1}{2\sqrt{x_0}}\epsilon_1 + \frac{1}{2\sqrt{x_0}}\epsilon_1 + \frac{-1}{4x_0^{3/2}}\epsilon_1$

Computing derivatives using bidual numbers – univariate example

- Consider a Taylor series expansion of the following bidual number

$$f(x+h(\epsilon_1+\epsilon_2)) = f(x) + h(\epsilon_1+\epsilon_2)f'(x) + \frac{h^2}{2!}(\epsilon_1+\epsilon_2)^2 f''(x) + H.O.T.$$

$$= f(x) + h((\epsilon_1+\epsilon_2)f'(x) + \frac{h^2}{2!}(\cancel{\epsilon_1^2}^{\,0} + 2\epsilon_1\epsilon_2 + \cancel{\epsilon_2^2}^{\,0})f''(x) + \cancel{H.O.T.}^{\,0}$$

$$= f(x) + h((\epsilon_1+\epsilon_2)f'(x) + \ h^2(\epsilon_1\epsilon_2)f''(x)$$

General case

$$f(x^*) = f\big(bidual(x_0, h_1, h_2, 0)\big)$$

$$\frac{df}{dx} = \frac{1}{h_1} Im_1(f(x^*)) = \frac{1}{h_2} Im_2(f(x^*))$$

$$\frac{d^2 f}{dx^2} = \frac{1}{h_1 h_2} Im_{12}(f(x^*))$$

Recommended: $h_1 = h_2 = 1$

$$f(x^*) = f\big(bidual(x_0, \overset{x_1}{1}, \overset{x_2}{1}, \overset{x_{12}}{0})\big)$$

$$\frac{df}{dx} = Im_1(f(x^*)) = Im_2(f(x^*))$$

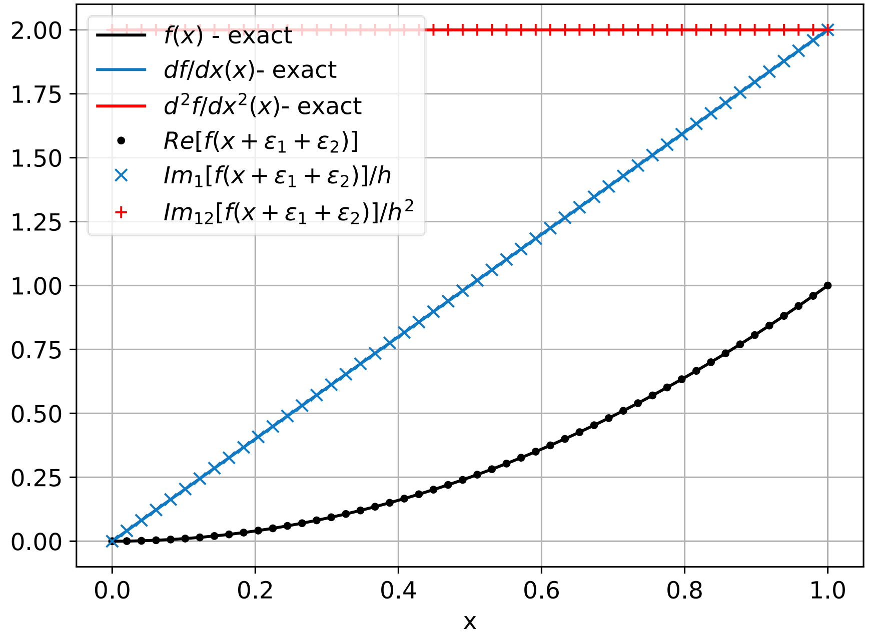
$$\frac{d^2 f}{dx^2} = Im_{12}(f(x^*))$$

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

- The use of bidual numbers to compute 1st and 2nd order derivatives can be demonstrated using some closed-form examples. All examples assume $h_1 = h_2 = 1$.

$$f(x) = x^2$$
$$f(x + \epsilon_1 + \epsilon_2) = (x + \epsilon_1 + \epsilon_2)^2 =$$
$$x^2 + 2x\epsilon_1 + 2x\epsilon_2 + 2\epsilon_1\epsilon_2 + \cancel{\epsilon_1^2}^{\,0} + \cancel{\epsilon_2^2}^{\,0}$$

$$\frac{df}{dx} = Im_1\big(f(x+\epsilon)\big) = Im_2\big(f(x+\epsilon)\big) = Im_1\big((x+\epsilon)^2\big) = 2x$$
$$\frac{d^2f}{dx^2} = Im_{12}\big(f(x+\epsilon)\big) = Im((x+\epsilon)^2) = 2$$



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

- The use of bidual numbers to compute 1st and 2nd order derivatives can be demonstrated using some closed-form examples. All examples assume $h_1 = h_2 = 1$.

$$f(x) = x^3$$

$$f(x + \epsilon_1 + \epsilon_2) = (x + \epsilon_1 + \epsilon_2)^3 =$$

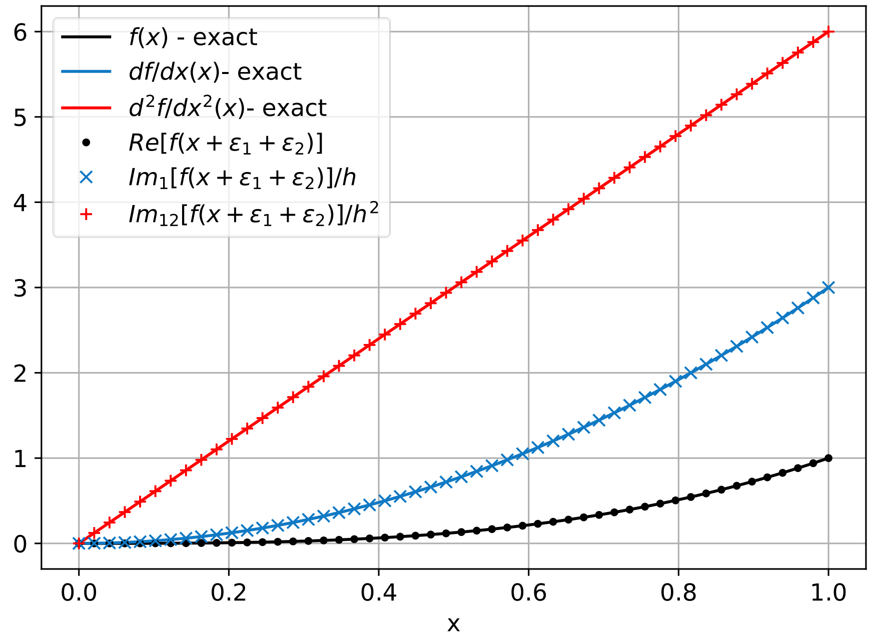
$$x^3 + 3x^2\epsilon_1 + 3x^2\epsilon_2 + 6x\epsilon_1\epsilon_2 + 3x\cancelto{0}{\epsilon_1^2} + 3x\cancelto{0}{\epsilon_2^2} + 3\epsilon_1\cancelto{0}{\epsilon_2^2} + 3\cancelto{0}{\epsilon_1^2}\epsilon_2 + \cancelto{0}{\epsilon_1^3} + \cancelto{0}{\epsilon_2^3}$$

$$= x^3 + 3x^2\epsilon_1 + 3x^2\epsilon_2 + 6x\epsilon_1\epsilon_2$$

$$\frac{df}{dx} = Im_1\big(f(x + \epsilon_1 + \epsilon_2)\big) = Im_2\big(f(x + \epsilon_1 + \epsilon_2)\big)$$

$$= Im_1\big((x + \epsilon_1 + \epsilon_2)^3\big) = 3x^2$$

$$\frac{d^2 f}{dx^2} = Im_{12}\big(f(x + \epsilon)\big) = Im\big((x + \epsilon)^3\big) = 6x$$



Closed-form example: $f(x) = e^x$

- The use of bidual numbers to compute 1st and 2nd order derivatives can be demonstrated using some closed-form examples. All examples assume $h_1 = h_2 = 1$.

$$f(x) = e^x$$

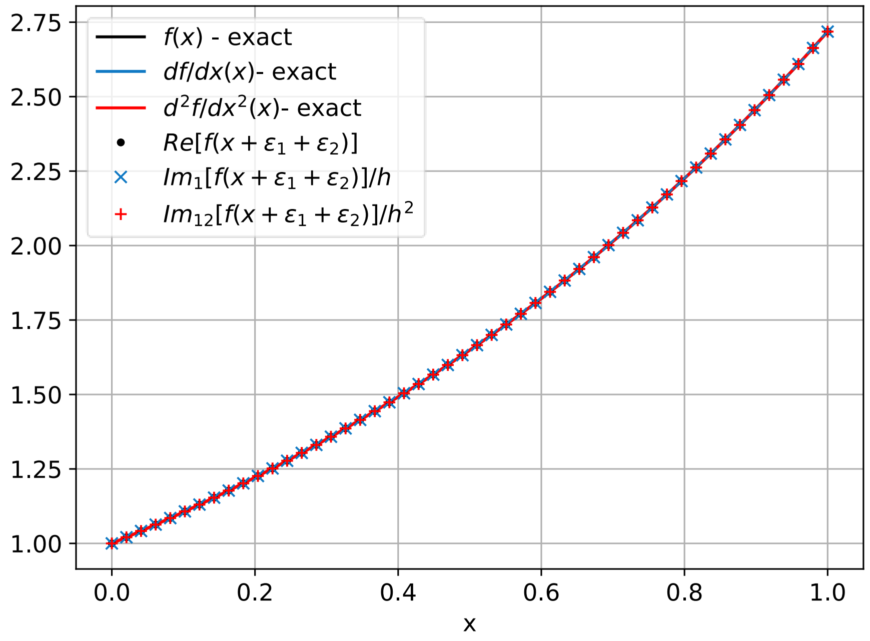
$$f(x + \epsilon_1 + \epsilon_2) = e^{x+\epsilon_1+\epsilon_2} =$$

$$e^x + e^x\epsilon_1 + e^x\epsilon_2 + e^x\epsilon_1\epsilon_2$$

$$\frac{df}{dx} = Im_1\big(f(x + \epsilon_1 + \epsilon_2)\big) = Im_2\big(f(x + \epsilon_1 + \epsilon_2)\big)$$

$$= Im_1(e^{x+\epsilon_1+\epsilon_2}) = e^x$$

$$\frac{d^2f}{dx^2} = Im_{12}\big(f(x + \epsilon)\big) = Im_{12}(e^{x+\epsilon_1+\epsilon_2}) = e^x$$



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

- The use of bidual numbers to compute 1st and 2nd order derivatives can be demonstrated using some closed-form examples. All examples assume $h_1 = h_2 = 1$.

$$f(x) = \sin(x)$$

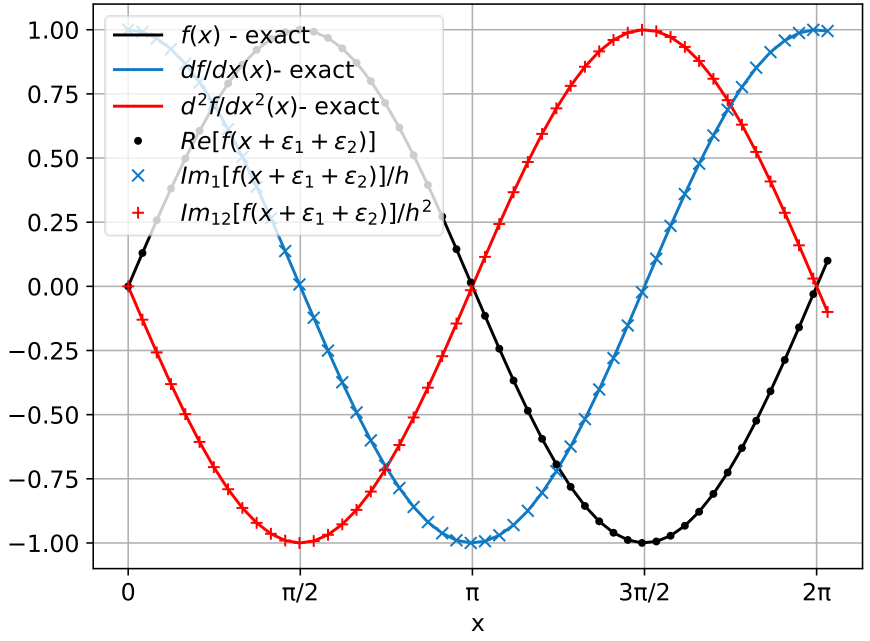
$$f(x+\epsilon_1+\epsilon_2) = \sin(x+\epsilon_1+\epsilon_2)$$

$$= \sin(x) + \cos(x)\,\epsilon_1 + \cos(x)\,\epsilon_2 - \sin(x)\epsilon_1\epsilon_2$$

$$\frac{df}{dx} = Im_1\big(f(x+\epsilon)\big) = Im_2\big(f(x+\epsilon)\big) = Im_1(\sin(x+\epsilon_1+\epsilon_2))$$

$$= \cos(x)$$

$$\frac{d^2f}{dx^2} = Im_{12}\big(f(x+\epsilon)\big) = Im_{12}(\sin(x+\epsilon_1+\epsilon_2)) = -\sin(x)$$



Closed-form example: $f(x) = \cos(x)$

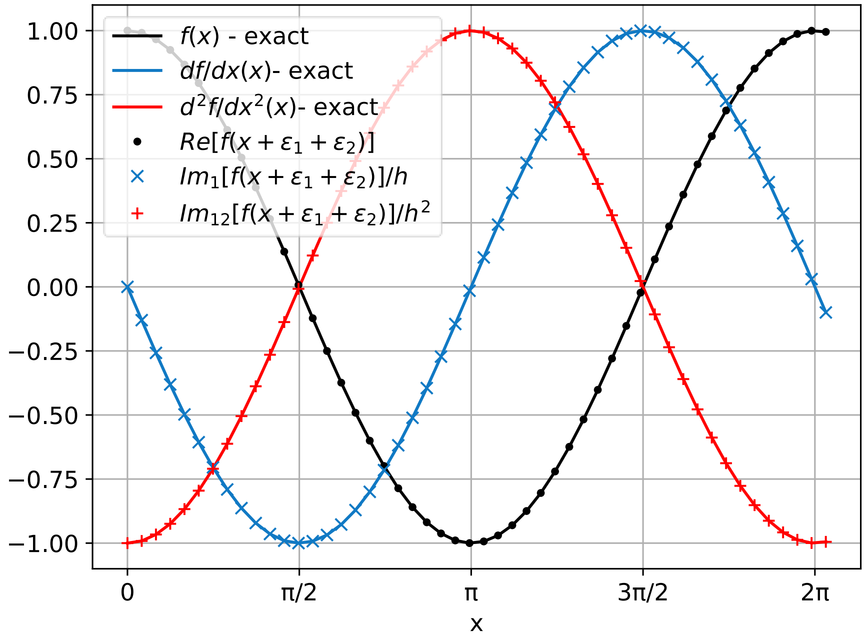
- The use of bidual numbers to compute 1st and 2nd order derivatives can be demonstrated using some closed-form examples. All examples assume $h_1 = h_2 = 1$.

$$f(x) = \cos(x)$$

$$f(x+\epsilon_1+\epsilon_2) = \cos(x+\epsilon_1+\epsilon_2)$$
$$= \sin(x) + \sin(x)\,\epsilon_1 + \sin(x)\,\epsilon_2 - \cos(x)\epsilon_1\epsilon_2$$

$$\frac{df}{dx} = Im_1\big(f(x+\epsilon)\big) = Im_2\big(f(x+\epsilon)\big) = Im_1(\cos(x+\epsilon_1+\epsilon_2))$$
$$= \sin(x)$$

$$\frac{d^2f}{dx^2} = Im_{12}\big(f(x+\epsilon)\big) = Im_{12}(\cos(x+\epsilon_1+\epsilon_2)) = -\cos(x)$$



Closed-form example: $f(x) = \ln(x)$

- The use of bidual numbers to compute 1st and 2nd order derivatives can be demonstrated using some closed-form examples. All examples assume $h_1 = h_2 = 1$.

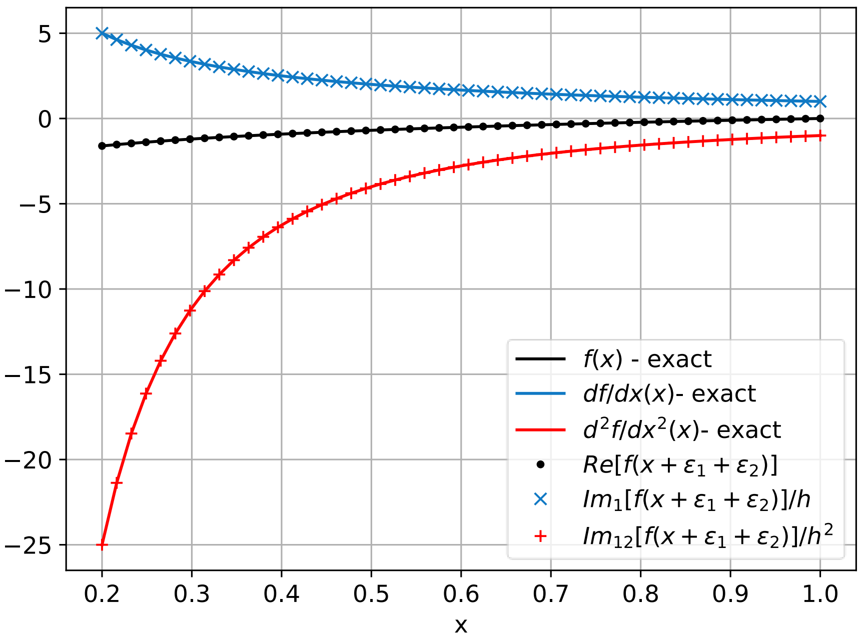
$$f(x) = \ln(x)$$

$$f(x+\epsilon_1+\epsilon_2) = \ln(x+\epsilon_1+\epsilon_2) = \frac{1}{x}\epsilon_1 + \frac{1}{x}\epsilon_2 - \frac{1}{x^2}\epsilon_{12}$$

$$\frac{df}{dx} = Im_1(\ln(x+\epsilon_1+\epsilon_2)) = Im_2(\ln(x+\epsilon_1+\epsilon_2))$$

$$= Im_1(\ln(x+\epsilon_1+\epsilon_2)) = \frac{1}{x}$$

$$\frac{d^2f}{dx^2} = Im_{12}\big(f(x+\epsilon_1+\epsilon_2)\big) = Im_{12}(\ln(x+\epsilon_1+\epsilon_2)) = -\frac{1}{x^2}$$



Computing derivatives using bidual numbers – <u>multivariate</u> example

- Consider a multivariate Taylor series expansion of the following bidual number

$$f(x + h\epsilon_1, y + h\epsilon_2) = f(x) + h(\epsilon_1 + \epsilon_2)f'(x) + \frac{h^2}{2!}(\epsilon_1 + \epsilon_2)^2 f''(x) + H.O.T.$$

$$= f(x) + h((\epsilon_1 + \epsilon_2)f'(x) + \frac{h^2}{2!}(\cancelto{0}{\epsilon_1^2} + 2\epsilon_1\epsilon_2 + \cancelto{0}{\epsilon_2^2})f''(x) + H.\cancelto{0}{O}.T.$$

$$= f(x) + h((\epsilon_1 + \epsilon_2)f'(x) + \ h^2(\epsilon_1\epsilon_2)f''(x)$$

<u>General Case: arbitrary h</u>

$$x^* = x + h\epsilon_1$$
$$y^* = y + h\epsilon_2$$
$$f(x^*, y^*) = f\big(bidual(x_0, \mathbf{h}, 0, 0), bidual(x_0, 0, \mathbf{h}, 0)\big)$$

$$\frac{df}{dx} = \frac{1}{h} Im_1(f(x^*, y^*))$$
$$\frac{df}{dy} = \frac{1}{h} Im_2(f(x^*, y^*))$$
$$\frac{\partial^2 f}{\partial x \partial y} = \frac{1}{h^2} Im_{12}(f(x^*, y^*))$$

Computing derivatives using bidual numbers – <u>multivariate</u> example

- Consider a multivariate Taylor series expansion of the following bidual number

$$f(x+h\epsilon_1, y+h\epsilon_2) = f(x) + h(\epsilon_1+\epsilon_2)f'(x) + \frac{h^2}{2!}(\epsilon_1+\epsilon_2)^2 f''(x) + H.O.T.$$

$$= f(x) + h((\epsilon_1+\epsilon_2)f'(x) + \frac{h^2}{2!}(\cancelto{0}{\epsilon_1^2} + 2\epsilon_1\epsilon_2 + \cancelto{0}{\epsilon_2^2})f''(x) + \cancelto{0}{H.O.T.}$$

$$= f(x) + h((\epsilon_1+\epsilon_2)f'(x) + h^2(\epsilon_1\epsilon_2)f''(x)$$

<u>Recommended: $h = 1$</u>

$$x^* = x + \epsilon_1$$
$$y^* = y + \epsilon_2$$
$$f(x^*, y^*) = f\big(bidual(x_0, \mathbf{1}, 0, 0), bidual(x_0, 0, \mathbf{1}, 0)\big)$$

$$\frac{df}{dx} = Im_1(f(x^*, y^*))$$
$$\frac{df}{dy} = Im_2(f(x^*, y^*))$$
$$\frac{\partial^2 f}{\partial x \partial y} = Im_{12}(f(x^*, y^*))$$

Closed-form example: $f(x, y) = xy$

- The use of bidual numbers to compute 1st and 2nd order derivatives can be demonstrated using some closed-form examples. All examples assume $h_1 = h_2 = 1$.

$$f(x, y) = xy$$
$$(x + \epsilon_1)(y + \epsilon_2) = xy + y\epsilon_1 + x\epsilon_2 + 1\epsilon_{12}$$

$$\frac{\partial f}{\partial x} = Im_1\left(f\left((x + \epsilon_1)(y + \epsilon_2)\right)\right) = y$$
$$\frac{\partial f}{\partial y} = Im_2\left(f\left((x + \epsilon_1)(y + \epsilon_2)\right)\right) = x$$

$$\frac{\partial^2 f}{\partial x \partial y} = Im_{12}\left(f\left((x + \epsilon_1)(y + \epsilon_2)\right)\right) = 1$$

Closed-form example: $f(x, y) = x^2y^2$

$$f(x,y) = x^2y^2$$
$$f((x+\epsilon_1),(y+\epsilon_2)) = (x+\epsilon_1)^2(y+\epsilon_2)^2 =$$
$$(x^2+2x\epsilon_1+\cancel{\epsilon_1^2}^{\,0})(y^2+2y\epsilon_2+\cancel{\epsilon_2^2}^{\,0}) =$$
$$= x^2y^2+2xy^2\epsilon_1+2x^2y\epsilon_2+4xy\epsilon_{12}$$

$$\frac{\partial f}{\partial x} = Im_1\left(f\left((x+\epsilon_1)(y+\epsilon_2)\right)\right) = 2xy^2$$
$$\frac{\partial f}{\partial y} = Im_2\left(f\left((x+\epsilon_1)(y+\epsilon_2)\right)\right) = 2x^2y$$

$$\frac{\partial^2 f}{\partial x \partial y} = Im_{12}\left(f\left((x+\epsilon_1)(y+\epsilon_2)\right)\right) = 4xy$$

Closed-form example: $f(x,y) = xe^y$

$$f(x,y) = x\,e^y$$
$$f\big((x+\epsilon_1),(y+\epsilon_2)\big) = (x+\epsilon_1)e^{y+\epsilon_2} =$$
$$xe^{y+\epsilon_2} + e^{y+\epsilon_2}\epsilon_1$$

$$But\ (\exp(x_0 + x_1\epsilon_1 + x_2\epsilon_2 + x_{12}\epsilon_{12})) =$$
$$exp(x_0) + x_1 exp(x_0)\epsilon_1 + x_2\, exp(x_0)\epsilon_2 + (x_1x_2 + x_{12})\exp(x_0)\epsilon_{12}$$

$$Then\ e^{y+\epsilon_2} = e^y + e^y\epsilon_2$$

$$(x+\epsilon_1)e^{y+\epsilon_2} = (x+\epsilon_1)(e^y + e^y\epsilon_{12}) =$$
$$xe^y + e^y\epsilon_1 + xe^y\epsilon_2 + e^y\epsilon_{12} =$$

$$\frac{\partial f}{\partial x} = Im_1\Big(f\big((x+\epsilon_1)(y+\epsilon_2)\big)\Big) = e^y$$
$$\frac{\partial f}{\partial y} = Im_2\Big(f\big((x+\epsilon_1)(y+\epsilon_2)\big)\Big) = xe^y$$
$$\frac{\partial^2 f}{\partial x\partial y} = Im_{12}\Big(f\big((x+\epsilon_1)(y+\epsilon_2)\big)\Big) = e^y$$

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Closed-form example: $f(x, y) = x\sin(y)$

$$f(x, y) = x\sin(y)$$
$$f\big((x+\epsilon_1),(y+\epsilon_2)\big) = (x+\epsilon_1)\sin(y+\epsilon_2)$$

$$But\ (\sin(x_0 + x_1\epsilon_1 + x_2\epsilon_2 + x_{12}\epsilon_{12})) =$$
$$sin(x_0) + x_1 cos(x_0)\epsilon_1 + x_2\ cos(x_0)\epsilon_2 + (x_{12}\ cos(x_0) - x_1x_2\ sin(x_0))\epsilon_{12}$$

$$Then\ \sin(y + 0\epsilon_1 + \epsilon_2 + 0\epsilon_{12}) = \sin(y) + 0\epsilon_1 + \cos(y)\epsilon_2 + 0\epsilon_{12}$$
$$and$$
$$(x+\epsilon_1)(\sin(y) + \cos(y))\epsilon_2 =$$
$$x\sin y + \sin(y)\,\epsilon_1 + x\cos(y)\,\epsilon_2 + \cos(y)\,\epsilon_{12}$$
$$\frac{\partial f}{\partial x} = Im_1\Big(f\big((x+\epsilon_1)(y+\epsilon_2)\big)\Big) = \sin(y)$$
$$\frac{\partial f}{\partial y} = Im_2\Big(f\big((x+\epsilon_1)(y+\epsilon_2)\big)\Big) = x\cos(y)$$
$$\frac{\partial^2 f}{\partial x \partial y} = Im_{12}\Big(f\big((x+\epsilon_1)(y+\epsilon_2)\big)\Big) = \cos(y)$$

UTSA

Closed-form example: $f(x,y) = x\sin(y)$

$$f(x,y) = x\sin(y)$$
$$f\big((x+\epsilon_1),(y+\epsilon_2)\big) = (x+\epsilon_1)\sin(y+\epsilon_2)$$

$$But\ (\sin(x_0 + x_1\epsilon_1 + x_2\epsilon_2 + x_{12}\epsilon_{12})) =$$
$$sin(x_0) + x_1 cos(x_0)\epsilon_1 + x_2\ cos(x_0)\epsilon_2 + (x_{12}\ cos(x_0) - x_1x_2\ sin(x_0))\epsilon_{12}$$

$$Then\ \sin(y + 0\epsilon_1 + \epsilon_2 + 0\epsilon_{12}) = \sin(y) + 0\epsilon_1 + \cos(y)\epsilon_2 + 0\epsilon_{12}$$
$$and$$
$$(x+\epsilon_1)(\sin(y) + \cos(y))\epsilon_2 =$$
$$x\sin y + \sin(y)\,\epsilon_1 + x\cos(y)\,\epsilon_2 + \cos(y)\,\epsilon_{12}$$
$$\frac{\partial f}{\partial x} = Im_1\Big(f\big((x+\epsilon_1)(y+\epsilon_2)\big)\Big) = \sin(y)$$
$$\frac{\partial f}{\partial y} = Im_2\Big(f\big((x+\epsilon_1)(y+\epsilon_2)\big)\Big) = x\cos(y)$$
$$\frac{\partial^2 f}{\partial x\partial y} = Im_{12}\Big(f\big((x+\epsilon_1)(y+\epsilon_2)\big)\Big) = \cos(y)$$

Incorrect method for computing derivatives using bidual numbers – <u>univariate</u> example

- What happens if we perturb $\epsilon_1, \epsilon_2, and\ \epsilon_{12}$? Consider a Taylor series expansion of the following bidual number

$$f(x + h(\epsilon_1 + \epsilon_2 + \epsilon_{12})) = f(x) + h(\epsilon_1 + \epsilon_2 + \epsilon_{12})f'(x) + \frac{h^2}{2!}(\epsilon_1 + \epsilon_2 + \epsilon_{12})^2 f''(x) + H.O.T.$$

$$= f(x) + h((\epsilon_1 + \epsilon_2 + \epsilon_{12})f'(x) + \frac{h^2}{2!}(\cancelto{0}{\epsilon_1^2} + 2\cancelto{0}{\epsilon_1\epsilon_{12}} + \cancelto{0}{\epsilon_{12}^2} + 2\epsilon_1\epsilon_2 + 2\cancelto{0}{\epsilon_{12}\epsilon_2} + \cancelto{0}{\epsilon_2^2})f''(x) + H.O.T.$$

$$= f(x) + hf'(x)\epsilon_1 + hf'(x)\epsilon_2 + (hf'(x) + h^2 f''(x))\epsilon_{12}$$

$$\boxed{\begin{aligned} &f(x^*) = f(x + h(\epsilon_1 + \epsilon_2 + \epsilon_{12})) \\ &Im_1(f(x^*)) = Im_2(f(x^*)) = h\frac{df}{dx} \\ &Im_{12}(f(x^*)) = h\frac{df}{dx} + h^2\frac{d^2f}{dx^2} \end{aligned}}$$

Convolve $f_{,x}$ and $f_{,xx}$

Incorrect method for computing derivatives using bidual numbers – univariate example

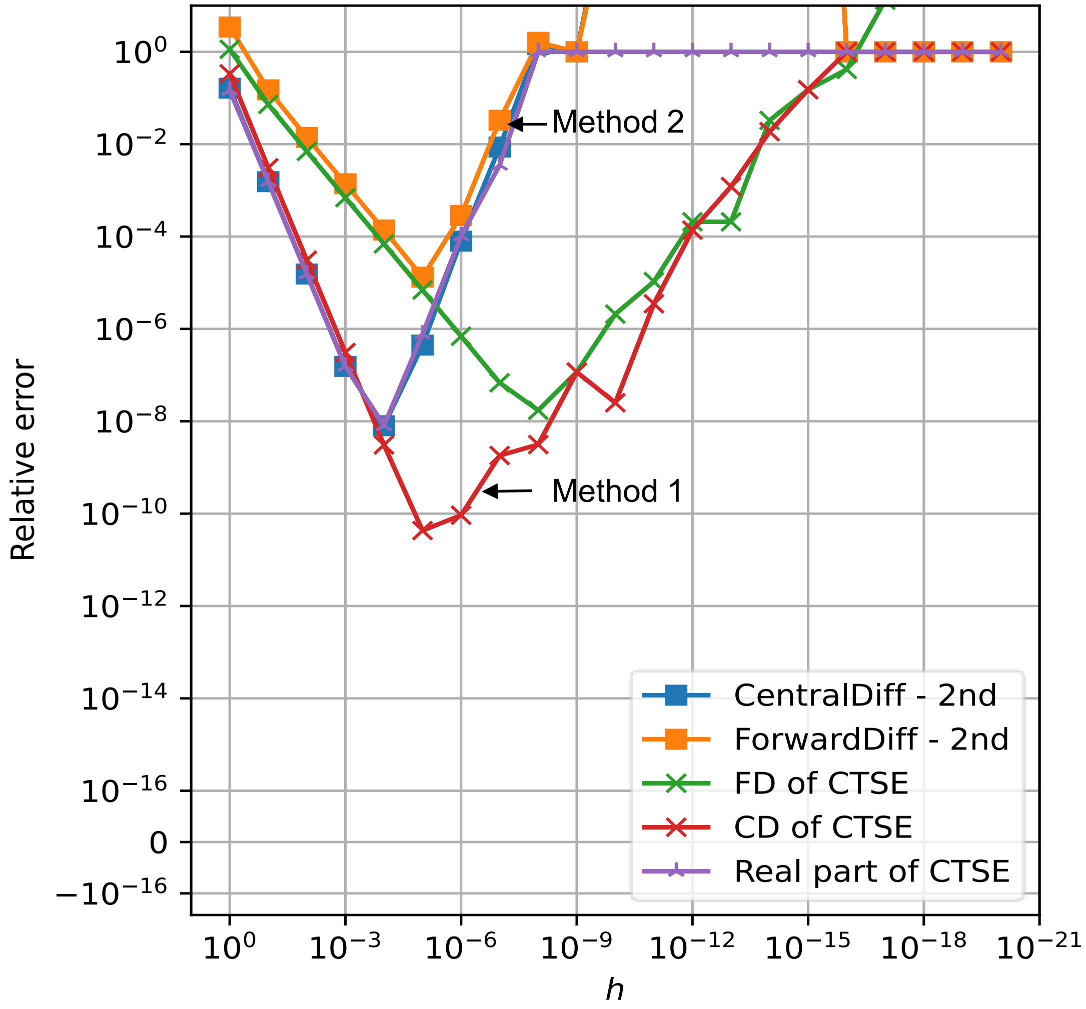
- How do we determine which non-real axes to perturb? Consider the following options – only case 4 provides the correct result.

$Case$	$Perturbation$	$Result$
1	$f(x+1\epsilon_1+0\epsilon_2+0\epsilon_{12})$	$f(x)+f_{,x}\epsilon_1+0\epsilon_2+0\epsilon_{12}$
2	$f(x+0\epsilon_1+1\epsilon_2+0\epsilon_{12})$	$f(x)+0\epsilon_1+f_{,x}\epsilon_2+0\epsilon_{12}$
3	$f(x+0\epsilon_1+0\epsilon_2+1\epsilon_{12})$	$f(x)+0\epsilon_1+0\epsilon_2+f_{,x}\epsilon_{12}$
4	$f(x+1\epsilon_1+1\epsilon_2+0\epsilon_{12})$	$\boldsymbol{f(x)+f_{,x}\epsilon_1+f_{,x}\epsilon_2+f_{,xx}\epsilon_{12}}$
5	$f(x+1\epsilon_1+0\epsilon_2+1\epsilon_{12})$	$f(x)+f_{,x}\epsilon_1+0\epsilon_2+f_{,x}\epsilon_{12}$
6	$f(x+0\epsilon_1+1\epsilon_2+1\epsilon_{12})$	$f(x)+0\epsilon_1+f_{,x}\epsilon_2+f_{,x}\epsilon_{12}$
7	$f(x+1\epsilon_1+1\epsilon_2+1\epsilon_{12})$	$f(x)+f_{,x}\epsilon_1+f_{,x}\epsilon_2+(f_{,x}+f_{,xx})\epsilon_{12}$

where $f_{,x}=\frac{df}{dx}, and\ f_{,xx}=\frac{d^2f}{dx^2}$

Step size study - $f(x) = sin(x)$

- Only bidual numbers can provide step-size independent 2nd order sensitivities.

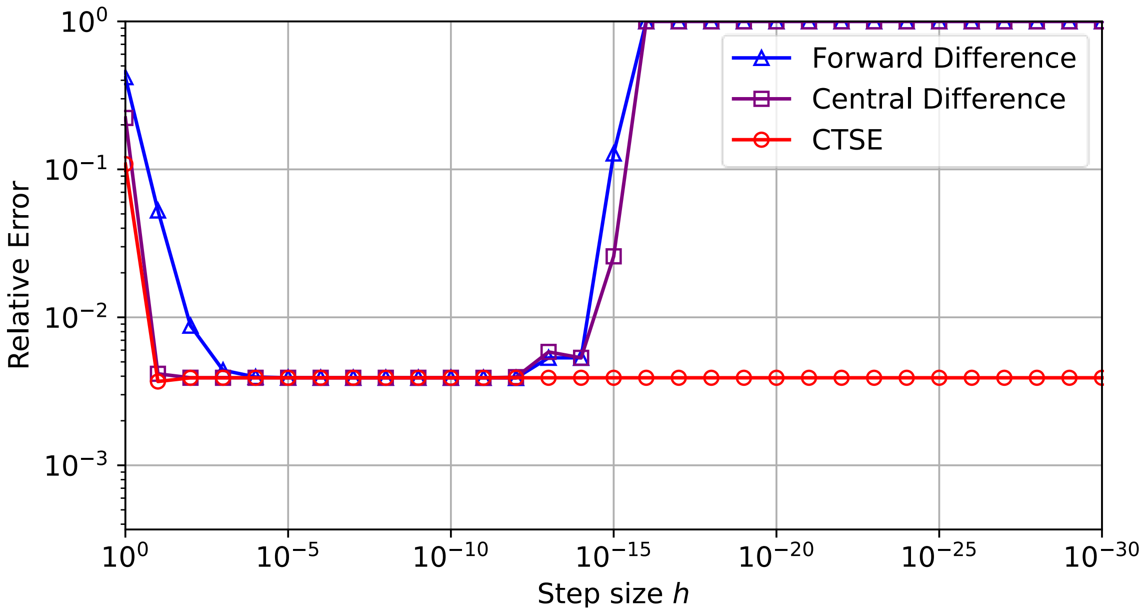


Show both 1st and 2nd order

Step size study – numerical integration

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

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



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

Both first and 2nd order

Application: Simpson's rule - $\frac{\partial^2 I}{\partial a^2}$

- Biduals can be used to calculate first and second derivatives of an integral using the Simpson's rule. Here we show 2nd order.

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: $\frac{\partial^2 I}{\partial a^2} = Im_{\epsilon_{12}}(I(a+\epsilon_1+\epsilon_2,b,c)$, replace a with $a+\epsilon_1+\epsilon_2$

$$I(a+\epsilon_1+\epsilon_2,b,c)$$
$$\approx \frac{b-(a+\epsilon_1+\epsilon_2)}{8}\left(f(a+\epsilon_1+\epsilon_2,c) + 3f\left(\frac{2(a+\epsilon_1+\epsilon_2)+b}{3},c\right) + 3f\left(\frac{(a+\epsilon_1+\epsilon_2)+2b}{3},c\right) + f(b,c)\right)$$

Then,

$$I = Re(I(a+\epsilon_1+\epsilon_2,b,c))$$

$$\frac{\partial I}{\partial a} = Im_{\epsilon_1}(I(a+\epsilon_1+\epsilon_2,b,c))$$

$$\frac{\partial I}{\partial b} = Im_{\epsilon_2}(I(a+\epsilon_1+\epsilon_2,b,c))$$

$$\frac{\partial^2 I}{\partial a^2} = Im_{\epsilon_{12}}(I(a+\epsilon_1+\epsilon_2,b,c))$$

Application: Simpson's rule - $\frac{\partial^2 I}{\partial b^2}$

To calculate: $\frac{\partial^2 I}{\partial b^2} = Im_{\epsilon_{12}}(I(a, b+\epsilon_1+\epsilon_2, c)$, replace b with $b+\epsilon_1+\epsilon_2$

$$I(a, b+\epsilon_1+\epsilon_2, c) \approx \frac{(b+\epsilon_1+\epsilon_2)-a}{8}\left(f(a,c) + 3f\left(\frac{2a+(b+\epsilon_1+\epsilon_2)}{3}, c\right) + 3f\left(\frac{a+2(b+\epsilon_1+\epsilon_2)}{3}, c\right) + f(b+\epsilon_1+\epsilon_2, c)\right)$$

Then,

$$I = Re(I(a, b+\epsilon_1+\epsilon_2, c))$$

$$\frac{\partial I}{\partial a} = Im_{\epsilon_1}(I(a, b+\epsilon_1+\epsilon_2, c))$$

$$\frac{\partial I}{\partial b} = Im_{\epsilon_2}(I(a, b+\epsilon_1+\epsilon_2, c))$$

$$\frac{\partial^2 I}{\partial a^2} = Im_{\epsilon_{12}}(I(a, b+\epsilon_1+\epsilon_2, c))$$

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Application: Simpson's rule - $\frac{\partial^2 I}{\partial c^2}$

To calculate: $\frac{\partial^2 I}{\partial c^2} = Im_{\epsilon_{12}}(I(a, b + \epsilon_1 + \epsilon_2, c + \epsilon_1 + \epsilon_2)$, replace b with$c + \epsilon_1 + \epsilon_2$

$$I(a, b, c + \epsilon_1 + \epsilon_2) \approx \frac{b-a}{8}\left(f(a, b, c + \epsilon_1 + \epsilon_2) + 3f\left(\frac{2a+b}{3}, c + \epsilon_1 + \epsilon_2\right) + 3f\left(\frac{a+2b}{3}, c + \epsilon_1 + \epsilon_2\right) + f(b, c + \epsilon_1 + \epsilon_2)\right)$$

Then,

$$I = Re(I(a, b, c + \epsilon_1 + \epsilon_2))$$

$$\frac{\partial I}{\partial a} = Im_{\epsilon_1}(I(a, b, c + \epsilon_1 + \epsilon_2))$$

$$\frac{\partial I}{\partial b} = Im_{\epsilon_2}(I(a, b, c + \epsilon_1 + \epsilon_2))$$

$$\frac{\partial^2 I}{\partial a^2} = Im_{\epsilon_{12}}(I(a, b, c + \epsilon_1 + \epsilon_2))$$

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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	Biduals	Relative Error
I	0.0786069	0.0785338	$9.3 * 10^{-4}$
$\partial^2 I/\partial a^2$	0.135335	0.131951	$2.5 * 10^{-2}$
$\partial^2 I/\partial b^2$	-0.0549469	-0.0554347	$8.9 * 10^{-3}$
$\partial^2 I/\partial c^2$	0.15887	0.15893	$3.7 * 10^{-4}$

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

The first order results are the same as when using CTSE and dual numbers.

Application: Simpson's rule - $\frac{\partial^2 I}{\partial a \partial b}$

- Biduals can be used to calculate first and mixed second derivatives of an integral using the Simpson's rule.

To calculate: $\frac{\partial^2 I}{\partial a \partial b} = Im_{\epsilon_{12}}(I(a+\epsilon_1, b+\epsilon_2, c)$, replace a with $a+\epsilon_1$ and b with $b+\epsilon_2$

Note, a and b can be perturbed using either ϵ_1 or ϵ_2, i.e.,

$$Im_{\epsilon_{12}}(I(a+\epsilon_1, b+\epsilon_2, c), = Im_{\epsilon_{12}}(I(a+\epsilon_2, b+\epsilon_1, c),$$

$$I(a+\epsilon_1, b+\epsilon_2, c) \approx \frac{(b+\epsilon_2)-(a+\epsilon_1)}{8}\left(f(a+\epsilon_1, c) + 3f\left(\frac{2(a+\epsilon_1)+(b+\epsilon_2)}{3}, c\right) + 3f\left(\frac{(a+\epsilon_1)+2(b+\epsilon_2)}{3}, c\right) + f(b+\epsilon_2, c)\right)$$

Then,

$$I = Re(I(a+\epsilon_1, b+\epsilon_2, c))$$

$$\frac{\partial I}{\partial a} = Im_{\epsilon_1}(I(a+\epsilon_1, b+\epsilon_2, c))$$

$$\frac{\partial I}{\partial b} = Im_{\epsilon_2}(I(a+\epsilon_1, b+\epsilon_2, c))$$

$$\frac{\partial^2 I}{\partial a \partial b} = Im_{\epsilon_{12}}(I(a+\epsilon_1, b+\epsilon_2, c))$$

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Application: Simpson's rule - $\frac{\partial^2 I}{\partial a \partial c}$

To calculate: $\frac{\partial^2 I}{\partial a \partial c} = Im_{\epsilon_{12}}(I(a+\epsilon_1, b, c+\epsilon_2)$, replace a with $a+\epsilon_1$ and c with $c+\epsilon_2$

$$I(a+\epsilon_1, b, c+\epsilon_2)$$
$$\approx \frac{b-(a+\epsilon_1)}{8}\left(f(a+\epsilon_1, c+\epsilon_2) + 3f\left(\frac{2(a+\epsilon_1)+b}{3}, c+\epsilon_2\right) + 3f\left(\frac{(a+\epsilon_1)+2b}{3}, c+\epsilon_2\right) + f(b, c+\epsilon_2)\right)$$

Then,

$$I = Re(I(a+\epsilon_1, b, c+\epsilon_2))$$

$$\frac{\partial I}{\partial a} = Im_{\epsilon_1}(I(a+\epsilon_1, b, c+\epsilon_2))$$

$$\frac{\partial I}{\partial c} = Im_{\epsilon_2}(I(a+\epsilon_1, b, c+\epsilon_2))$$

$$\frac{\partial^2 I}{\partial a \partial c} = Im_{\epsilon_{12}}(I(a+\epsilon_1, b, c+\epsilon_2))$$

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Application: Simpson's rule - $\frac{\partial^2 I}{\partial b \partial c}$

To calculate: $\frac{\partial^2 I}{\partial b \partial c} = Im_{\epsilon_{12}}(I(a, b+\epsilon_1, c+\epsilon_2)$, replace b with $b+\epsilon_1$ and c with $c+\epsilon_2$

$$I(a, b+\epsilon_1, c+\epsilon_2)$$
$$\approx \frac{(b+\epsilon_1)-a}{8}\left(f(a, c+\epsilon_2) + 3f\left(\frac{2a+(b+\epsilon_1)}{3}, c+\epsilon_2\right) + 3f\left(\frac{a+2(b+\epsilon_1)}{3}, c+\epsilon_2\right) + f(b+\epsilon_1, c+\epsilon_2)\right)$$

Then,
$$I = Re(I(a, b+\epsilon_1, c+\epsilon_2))$$
$$\frac{\partial I}{\partial b} = Im_{\epsilon_1}(I(a, b+\epsilon_1, c+\epsilon_2))$$

$$\frac{\partial I}{\partial c} = Im_{\epsilon_2}(I(a, b+\epsilon_1, c+\epsilon_2))$$
$$\frac{\partial^2 I}{\partial b \partial c} = Im_{\epsilon_{12}}(I(a, b+\epsilon_1, c+\epsilon_2))$$

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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	Simpson's Rule	Relative Error
Integral	0.0786069	0.0785338	$9.3 * 10^{-4}$
$\partial^2 I/\partial a \partial b$	0.0000	0.00152859	$1.5 * 10^{-3\dagger}$
$\partial^2 I/\partial a \partial c$	0.135335	0.134908	$3.2 * 10^{-3}$
$\partial^2 I/\partial b \partial c$	-0.0732626	-0.0728604	$5.5 * 10^{-3}$

† Absolute error

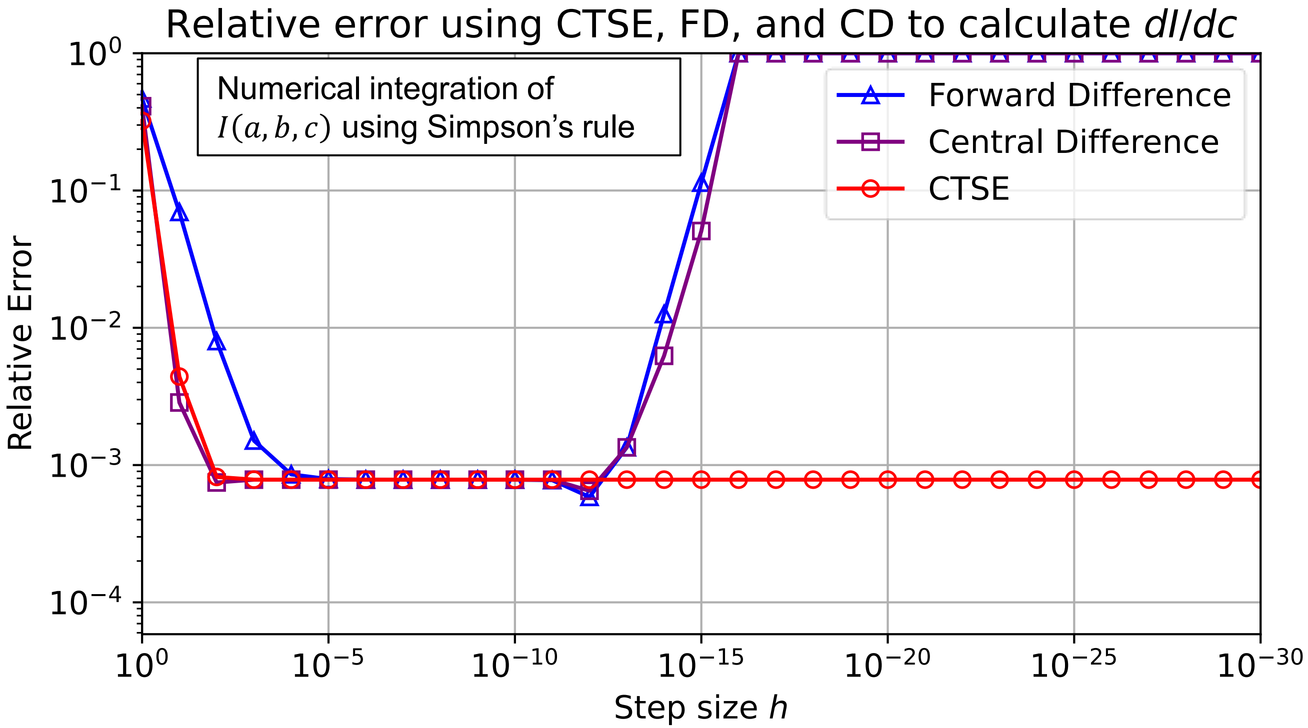
Note that the accuracy of the derivatives are ~one order of magnitude less than the integral. This behavior is often seen in other applications.

The first order results are the same as when using CTSE and dual numbers.

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 $a = 1, b = 2, c = 2$



Update for 2nd order.

Application: Simpson's rule

- Compare the accuracy of $\partial^2 I/\partial c^2$ computed 2 ways: 1)Bidual numbers applied directly to I, and 2) Integration of the analytical equation. Both integrals computed using Simpson's rule.

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

$$\frac{\partial^2 I_1}{\partial c^2} \approx Im(I(a,b,c + \epsilon_1 + \epsilon_2)) \qquad \frac{\partial^2 I_1}{\partial c^2} = \frac{\partial}{\partial c^2}\int_a^b xe^{-cx}dx = \int_a^b \frac{\partial^2}{\partial c^2}(xe^{-cx})dx = \int_a^b (x^3 e^{-cx})dx$$

Biduals	Analytical derivative
$\frac{\partial^2 I_1}{\partial c^2} \approx Im(I(a,b,c + \epsilon_1 + \epsilon_2))$	$\frac{d^2 I_2}{dc^2} = \int_a^b (x^3 e^{-cx})dx$
0.158929633274781	0.158929633274781

To summarize, Biduals provide the most accurate derivative possible – 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: $dI/da \approx \frac{Im(I(a+ih,b,c)}{h}$, 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	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	$1.27 * 10^{-5}$

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

Application: Gauss-Legendre quadrature

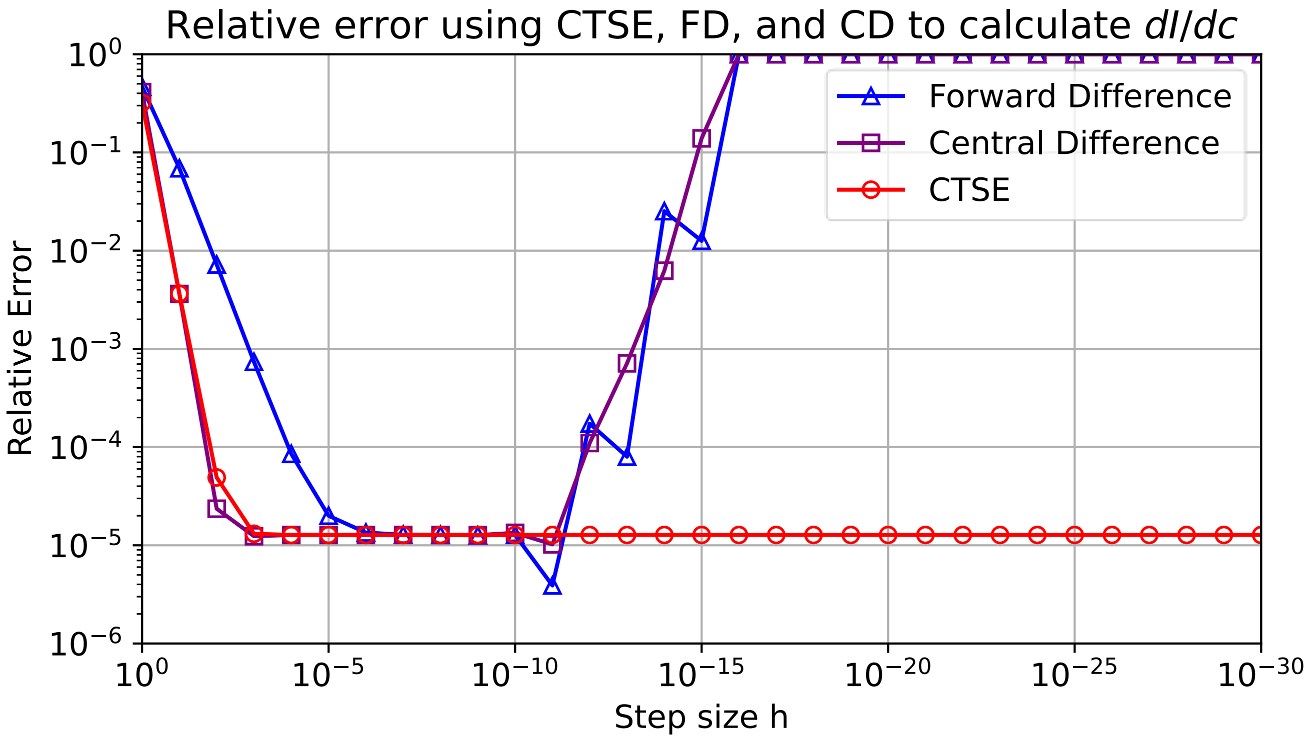
- Example: $I(a,b,c) = \int_a^b xe^{-cx}dx$ with $a = 1, b = 2, c = 2$

	Exact	Biduals	Relative Error
I	0.0786069	0.0785338	$9.3 * 10^{-4}$
$\partial^2 I/\partial a^2$	0.135335	0.135495	$1.2 * 10^{-3}$
$\partial^2 I/\partial b^2$	-0.0549469	-0.0548812	$1.2 * 10^{-3}$
$\partial^2 I/\partial c^2$	0.15887	0.158867	$1.8 * 10^{-5}$

The first order results are the same as when using CTSE and dual numbers.

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.

Application: Gauss-Legendre quadrature

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

	Exact	Simpson's Rule	Relative Error
Integral	0.0786069	0.0785338	$9.3 * 10^{-4}$
$\partial^2 I/\partial a \partial b$	0.0000	-0.0001044	$1.0 * 10^{-4\dagger}$
$\partial^2 I/\partial a \partial c$	0.135335	0.135321	$1.0 * 10^{-4}$
$\partial^2 I/\partial b \partial c$	-0.0732626	-0.0732562	$8.6 * 10^{-5}$

† Absolute error

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

The first order results are the same as when using CTSE and dual numbers.

Example: Newton-Raphson Method– multivariate example

- Consider the vector valued function:

$$f(x,y) = \begin{cases} x^2 + y^2 - 4 \\ 4x^2 - y^2 - 4 \end{cases}$$

- Suppose we want to find where $f(x,y) = 0$. To solve, we implement multivariate Newton-Raphson method

$$\boldsymbol{x}_k = \boldsymbol{x}_{k-1}[Df(\boldsymbol{x}_{k-1})]f(\boldsymbol{x}_{k-1})$$

Use J for Jacobian?

- Here Df represents the Jacobian matrix of the function f

Example: Newton-Raphson Method– multivariate example

- Let $f(x,y) = \begin{cases} f_1(x,y) \\ f_2(x,y) \end{cases}$
- Recall Df is given by: $\begin{bmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_1}{\partial y} \\ \frac{\partial f_2}{\partial x} & \frac{\partial f_2}{\partial x} \end{bmatrix}$

We can find $\frac{\partial f_1}{\partial x}, \frac{\partial f_1}{\partial y}, \frac{\partial f_2}{\partial x}, \frac{\partial f_2}{\partial x}$ using bidual numbers so that:

$$\frac{\partial f_1}{\partial x} = Im_1\big(f_1(x+\ \varepsilon, y+\ \epsilon)\big), \qquad \frac{\partial f_1}{\partial y} = Im_2(f_1(x+\ \varepsilon, y+\ \epsilon))$$
$$\frac{\partial f_2}{\partial x} = Im_1\big(f_2(x+\ \varepsilon, y+\ \epsilon)\big), \qquad \frac{\partial f_2}{\partial y} = Im_2(f_1(x+\ \varepsilon, y+\ \epsilon))$$

Example: Newton-Raphson Method– multivariate example

Suggest we show the intermediate calculations in some form for users to follow & verify their code

Iteration no.	x	y	Jx	Jy	Relative Error X	Relative Error Y

Example: Newton-Raphson Method– multivariate example

- Using this approach, we arrive at the solution:

$$x^* = 1.2649110640673549$$
$$y^* = 1.549193338549693$$

Align x* and y*

- Note that:

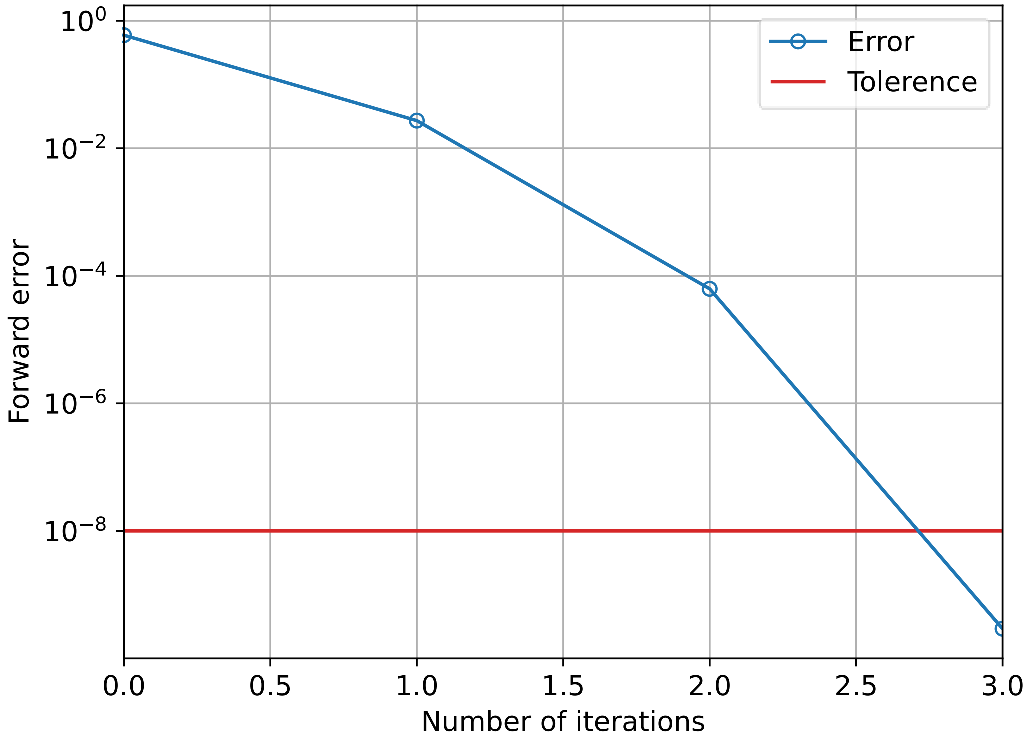
$$f(x^*, y^*) = \begin{pmatrix} 2.06751949e^{-10} \\ -2.06712425e^{-10} \end{pmatrix}$$

- This solution is within an acceptable tolerance for solving the problem $f(x, y) = 0$

Example: Newton-Raphson Method– multivariate example

- A plot showing the number of iterations versus the relative error of the Newton-Raphson method using bidual numbers. This example converges after just three iterations.

What does ”forward error” mean. Should we use “Relative error”?



ODE solver – Euler's method with bidual numbers

- Using bidual numbers, in a single analysis compute either: a) 1st and 2nd order derivatives with respect to a single variable, or b) 1st and 2nd order *mixed* derivatives can be computed of two variables. As examples:
  - a) Compute $\frac{\partial I}{\partial a}, \frac{\partial^2 I}{\partial a^2}$.

    or
  - b) Compute $\frac{\partial I}{\partial a}, \frac{\partial I}{\partial b}, \frac{\partial^2 I}{\partial a \partial b}$.

$$y'(x) = ay(x) + bx - x^2 \qquad\qquad y(0) = g$$
$$a = 1, b = 2, g = 1$$

ODE solver – Euler's method with bidual numbers

- Exact solutions ($a = 1, b = 2\ g = 1$)

First Order

$\frac{\partial y}{\partial a}$	$-2 - 2x - x^2 + (2 + x)e^x$
$\frac{\partial y}{\partial b}$	$-1 - x + e^x$
$\frac{\partial y}{\partial g}$	e^x

Second Order

$\frac{\partial^2 y}{\partial a^2}$	$e^x(-12 + 4x + x^2)$ $+2(6 + 4x + x^2)$
$\frac{\partial^2 y}{\partial b^2}$	0
$\frac{\partial^2 y}{\partial g^2}$	0

Mixed Second Order

$\frac{\partial^2 y}{\partial a \partial b}$	$e^x(x - 2) + x + 2$
$\frac{\partial^2 y}{\partial a \partial g}$	xe^x
$\frac{\partial^2 y}{\partial b \partial g}$	0

UTSA

ODE solver – Euler's method

- The numerical results using Euler's method are shown below using a step size of $h_{ode} = 0.1$.

$$y'(x) = f(x, y) = ay(x) + bx - x^2$$

$$y(0) = g$$

$$a = 1, b = 2, g = 1$$

Euler's method:

$$y_{i+1}(x) = y_i + y'(x)h_{ode}$$

$$y'(x) = 1y(x) + 2x - x^2$$
$$y_0(0) = 1$$
$$h_{ode} = 0.1$$

h_{ode} is the step size used for Euler's method – this is independent from the h used by biduals.

Numerical solution for y:

X	y_i	$y'(x)$	y_{i+1}	y_{exact}	Relative Error
0.0	1.0	1.0	1.1	1.0	---
0.1	1.1	1.129	1.290	1.1152	$9.80 * 10^{-2}$
0.2	1.229	1.589	1.388	1.2614	$1.09 * 10^{-1}$
0.3	1.388	1.898	1.578	1.4399	$1.20 * 10^{-1}$
0.4	1.578	2.218	1.799	1.6518	$1.29 * 10^{-1}$

ODE solver – $dy(x)/da$ and $d^2y(x)/da^2$ results

- The sensitivities $dy(x)/da$ and $d^2y(x)/da^2$ can be obtained using the standard Euler's method but now with a is replaced by $a + \epsilon_1 + \epsilon_2$ and the derivatives are obtained as $\frac{dy(x)}{da} \approx Im_1(y(x)), \frac{d^2y(x)}{da^2} \approx Im_{12}(y(x))$.

$$y'(x) = (1 + \epsilon_1 + \epsilon_2)y(x) + 2x - x^2 \text{ with } y(0) = 1$$

X	dy/da	dy/da Exact	Relative Error	d^2y/da^2	d^2y/da^2 Exact	Relative Error
0.0	1.0	0	---	0	0	0
0.1	0.1	0.1108	$9.80 * 10^{-2}$	0	0.0111	1
0.2	0.22	0.2471	$1.09 * 10^{-1}$	0.0200	0.0491	$5.93 * 10^{-1}$
0.3	0.3649	0.4147	$1.20 * 10^{-1}$	0.0660	0.1230	$4.64 * 10^{-1}$
0.4	0.5402	0.6204	$1.29 * 10^{-1}$	0.1456	0.2437	$4.03 * 10^{-1}$

ODE solver – $dy(x)/db$ and $d^2y(x)/db^2$ results

- The sensitivities $dy(x)/db$ and $d^2y(x)/db^2$ can be obtained using the standard Euler's method but now with b is replaced by $b+\epsilon_1+\epsilon_2$ and the derivatives are obtained as $\frac{dy(x)}{db} \approx Im_1\big(y(x)\big), \frac{d^2y(x)}{db^2} \approx Im_{12}\big(y(x)\big)$.

$$y'(x) = y(x) + (2+\epsilon_1+\epsilon_2)x - x^2 \text{ with } y(0) = 1$$

X	dy/db	dy/db Exact	Relative Error	d^2y/db^2	d^2y/db^2 Exact	Relative Error
0.0	1.0	0	---	0	0	0
0.1	0.1	0.1108	$9.80 * 10^{-2}$	0	0	0
0.2	0.22	0.2471	$1.09 * 10^{-1}$	0	0	0
0.3	0.3649	0.4147	$1.20 * 10^{-1}$	0	0	0
0.4	0.5402	0.6204	$1.29 * 10^{-1}$	0	0	0

ODE solver – $dy(x)/dg$ and $d^2y(x)/dg^2$ results

- The sensitivities $dy(x)/dg$ and $d^2y(x)/dg^2$ can be obtained using the standard Euler's method but now with g is replaced by $g+\epsilon_1+\epsilon_2$ and the derivatives are obtained as $\frac{dy(x)}{dg} \approx Im_1\big(y(x)\big), \frac{d^2y(x)}{dg^2} \approx Im_{12}\big(y(x)\big)$.

$$y'(x) = 1y(x) + 2x - x^2 \text{ with } y(0) = 1+\epsilon_1+\epsilon_2$$

X	dy/dg	dy/dg Exact	Relative Error	d^2y/dg^2	d^2y/dg^2 Exact	Relative Error
0.0	1.0	0	---	0	0	0
0.1	0.1	0.1108	$9.80*10^{-2}$	0	0	0
0.2	0.22	0.2471	$1.09*10^{-1}$	0	0	0
0.3	0.3649	0.4147	$1.20*10^{-1}$	0	0	0
0.4	0.5402	0.6204	$1.29*10^{-1}$	0	0	0

ODE solver – mixed derivative $\frac{\partial^2 y(x)}{\partial a \partial b}$

- The sensitivities $\partial y(x)/\partial a$, $\partial y(x)/\partial b$ and $\partial^2 y(x)/\partial a \partial b$ can be obtained using the standard Euler's method but now with a is replaced by $a + \epsilon_1$ and b is replaced by $b + \epsilon_2$. The derivatives are obtained as $\frac{\partial y(x)}{\partial a} \approx Im_1(y(x)), \frac{\partial y(x)}{\partial b} \approx Im_2(y(x)), \frac{\partial^2 y(x)}{\partial a \partial b} \approx Im_{12}(y(x))$.

$y'(x) = (1 + \epsilon_1)y(x) + (2 + \epsilon_2)x - x^2$ with $y(0) = 1$

X	$\partial^2 y/\partial a \partial b$	$\partial^2 y/\partial a \partial b$ Exact	Relative Error
0.0	0	0	0
0.1	0	.00018	1
0.2	0	.00148	1
0.3	.001	.00524	$8.09 * 10^{-1}$
0.4	.0042	.01308	$6.79 * 10^{-1}$

Equivalent forms	
$a + \epsilon_1$	$b + \epsilon_2$
$a + \epsilon_2$	$b + \epsilon_1$

Note, either ϵ_1 or ϵ_2 can be used to perturb a or b, that is .

ODE solver – mixed derivative $\frac{\partial^2 y(x)}{\partial a \partial b}$

- The sensitivities $\partial y(x)/\partial a$, $\partial y(x)/\partial b$ and $\partial^2 y(x)/\partial a \partial b$ can be obtained using the standard Euler's method but now with a is replaced by $a + \epsilon_1$ and b is replaced by $b + \epsilon_2$. The derivatives are obtained as $\frac{\partial y(x)}{\partial a} \approx Im_1\big(y(x)\big), \frac{\partial y(x)}{\partial b} \approx Im_2\big(y(x)\big), \frac{\partial^2 y(x)}{\partial a \partial b} \approx Im_{12}(y(x))$.

$$y'(x) = (1 + \epsilon_1)y(x) + (2 + \epsilon_2)x - x^2 \text{ with } y(0) = 1$$

X	$\partial^2 y/\partial a \partial b$	$\partial^2 y/\partial a \partial b$ Exact	Relative Error
0.0	0	0	0
0.1	0	.00018	1
0.2	0	.00148	1
0.3	.001	.00524	$8.09 * 10^{-1}$
0.4	.0042	.01308	$6.79 * 10^{-1}$

ODE solver – mixed derivative $\frac{\partial^2 y(x)}{\partial b \partial g}$

- The sensitivities $\partial y(x)/\partial b$, $\partial y(x)/\partial g$ and $\partial^2 y(x)/\partial b\partial g$ can be obtained using the standard Euler's method but now with b is replaced by $b+\epsilon_1$ and g is replaced by $g+\epsilon_2$. The derivatives are obtained as $\frac{\partial y(x)}{\partial b} \approx Im_1\big(y(x)\big), \frac{\partial y(x)}{\partial g} \approx Im_2\big(y(x)\big), \frac{\partial^2 y(x)}{\partial b\partial g} \approx Im_{12}(y(x))$.

$$y'(x) = y(x) +_* (2+\epsilon_1)x - x^2 \text{ with } y(0) = 1+\epsilon_2$$

X	$\partial^2 y/\partial b\partial g$	$\partial^2 y/\partial b\partial g$ Exact	Relative Error
0.0	0	0	0
0.1	0	0	0
0.2	0	0	0
0.3	0	0	0
0.4	0	0	0

ODE solver – mixed derivative $\frac{\partial^2 y(x)}{\partial a \partial g}$

- Equivalent results can be obtained for all cases by perturbing a along ϵ_2 and b along ϵ_1.The sensitivities can be obtained with a is replaced by $a+\epsilon_2$ and g is replaced by $g+\epsilon_1$. The derivatives are obtained as $\frac{\partial y(x)}{\partial a} \approx Im_2\big(y(x)\big), \frac{\partial y(x)}{\partial g} \approx Im_1\big(y(x)\big), \frac{\partial^2 y(x)}{\partial a \partial g} \approx Im_{12}(y(x))$.

$$y'(x) = (1+\epsilon_2)y(x) + 2x - x^2 \text{ with } y(0) = 1+\epsilon_1$$

X	$\partial^2 y/\partial a \partial g$	$\partial^2 y/\partial a \partial g$ Exact	Relative Error
0.0	0	0	0
0.1	0.1000	0.1105	$9.52 * 10^{-2}$
0.2	0.2200	0.2443	$9.94 * 10^{-2}$
0.3	0.3630	0.4050	$1.04 * 10^{-1}$
0.4	0.5324	0.5967	$1.08 * 10^{-1}$

Cauchy-Reimann form of biduals

- Bidual numbers have an equivalent CR form consisting of a matrix of all real coefficients.
- In this form there are no imaginary numbers and matrix operations can be used to manipulate the bidual numbers.

$$x_0 + x_1\epsilon_1 + x_2\epsilon_2 + x_{12}\epsilon_{12} = \begin{pmatrix} x_0 & 0 & 0 & 0 \\ x_1 & x_0 & 0 & 0 \\ x_2 & 0 & x_0 & 0 \\ x_{12} & x_2 & x_1 & x_0 \end{pmatrix}$$

Operations using CR form - Multiplication

- Consider the multiplication of two bidual numbers using the CR form

$$x^* = x_0 + x_1\epsilon_1 + x_2\epsilon_2 + x_{12}\epsilon_{12} \qquad y^* = y_0 + y_1\epsilon_1 + y_2\epsilon_2 + y_{12}\epsilon_{12}$$

$$x^* * y^* = \begin{pmatrix} x_0 & 0 & 0 & 0 \\ x_1 & x_0 & 0 & 0 \\ x_2 & 0 & x_0 & 0 \\ x_{12} & x_2 & x_1 & x_0 \end{pmatrix} \begin{pmatrix} y_0 & 0 & 0 & 0 \\ y_1 & y_0 & 0 & 0 \\ y_2 & 0 & y_0 & 0 \\ y_{12} & x_2 & y_1 & y_0 \end{pmatrix}$$

$$= \begin{pmatrix} x_0 y_0 & 0 & 0 & 0 \\ x_1 y_0 + a_0 y_1 & x_0 y_0 & 0 & 0 \\ x_2 y_0 + a_0 y_2 & 0 & x_0 y_0 & 0 \\ x_0 y_{12} + x_1 y_2 + x_2 y_1 + x_{12} y_0 & x_1 y_0 + x_0 y_1 & x_2 y_0 + x_0 y_2 & x_0 y_0 \end{pmatrix}$$

Operations using CR form - Division

- Consider a bidual number divided by a bidual number using the CR form

$$x^* = x_0 + x_1\epsilon_1 + x_2\epsilon_2 + x_{12}\epsilon_{12} \qquad y^* = y_0 + y_1\epsilon_1 + y_2\epsilon_2 + y_{12}\epsilon_{12}$$

$$\frac{x^*}{y^*} = \begin{pmatrix} x_0 & 0 & 0 & 0 \\ x_1 & x_0 & 0 & 0 \\ x_2 & 0 & x_0 & 0 \\ x_{12} & x_2 & x_1 & x_0 \end{pmatrix} \begin{pmatrix} y_0 & 0 & 0 & 0 \\ y_1 & y_0 & 0 & 0 \\ y_2 & 0 & y_0 & 0 \\ y_{12} & x_2 & y_1 & y_0 \end{pmatrix}^{-1}$$

$$= \begin{pmatrix} x_0/y_0 & 0 & 0 & 0 \\ x_1/y_0 - x_0 y_1/y_0^2 & x_0/y_0 & 0 & 0 \\ x_2/y_0 - x_0 y_2/y_0^2 & 0 & x_0/y_0 & 0 \\ x_{12}/y_0 - x_2 y_1/y_0^2 - x_1 y_2/y_0^2 - x_0(2y_0 y_1 y_2 - y_{12} y_0^2)/y_0^4 & x_1/y_0 - x_0 y_1/y_0^2 & x_2/y_0 - x_0 y_2/y_0^2 & x_0/y_0 \end{pmatrix}$$

Functions of Bidual numbers using the CR form

- Functions of bidual numbers can be computed using the CR form if one uses **functions of matrices**.

$$x^* = x_0 + x_1\epsilon_1 + x_2\epsilon_2 + x_{12}\epsilon_{12}$$

$$\exp(x^*) = \exp[\begin{pmatrix} x_0 & 0 & 0 & 0 \\ x_1 & x_0 & 0 & 0 \\ x_2 & 0 & x_0 & 0 \\ x_{12} & x_2 & x_1 & x_0 \end{pmatrix}]$$

$$= \begin{pmatrix} e^{x_0} & 0 & 0 & 0 \\ x_1 e^{x_0} & e^{x_0} & 0 & 0 \\ x_2 e^{x_0} & 0 & e^{x_0} & 0 \\ (x_1 x_2 + x_{12})e^{x_0} & x_1 e^{x_0} & x_2 e^{x_0} & e^{x_0} \end{pmatrix}$$

Computing derivatives using Bidual numbers using the CR form – general univariate example

- To use bidual numbers to compute derivatives with the CR form, perturb x along ϵ_1 and ϵ_2, i.e.,

$$x^* = x_0 + h_1\epsilon_1 + h_2\epsilon_2$$

$$[x^*] = \begin{bmatrix} x_0 & 0 & 0 & 0 \\ h_1 & x_0 & 0 & 0 \\ h_2 & 0 & x_0 & 0 \\ 0 & h_2 & h_1 & x_0 \end{bmatrix}$$

$$f([x^*]) = f\left(\begin{bmatrix} x_0 & 0 & 0 & 0 \\ h_1 & x_0 & 0 & 0 \\ h_2 & 0 & x_0 & 0 \\ 0 & h_2 & h_1 & x_0 \end{bmatrix}\right) =$$

$$\begin{bmatrix} f(x_0) & 0 & 0 & 0 \\ h_1\partial f(x_0)/\partial x & f(x_0) & 0 & 0 \\ h_2\partial f(x_0)/\partial x & 0 & f(x_0) & 0 \\ h_1h_2\partial^2 f(x_0)/\partial x^2 & h_2\partial f(x_0)/\partial x & h_1\partial f(x_0)/\partial x & f(x_0) \end{bmatrix}$$

$$\boxed{\begin{gathered} f(x_0) = f([x^*])_{11} \\ \partial f(x_0)/\partial x = \frac{1}{h_1} f([x^*])_{21} = \frac{1}{h_2} f([x^*])_{31} \\ \partial^2 f(x_0)/\partial x^2 = \frac{1}{h_1h_2} f([x^*])_{41} \end{gathered}}$$

Computing derivatives using Bidual numbers using the CR form – recommended <u>univariate</u> example

- It is recommended that we use $h_1 = h_2 = 1$ and the method simplifies to,

$$x^* = x + \epsilon_1 + \epsilon_2 \qquad [x^*] = \begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 1 & 0 & x_0 & 0 \\ 0 & 1 & 1 & x_0 \end{bmatrix}$$

$$f([x^*]) = f\left(\begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 1 & 0 & x_0 & 0 \\ 0 & 1 & 1 & x_0 \end{bmatrix}\right) =$$

$$\begin{bmatrix} f(x_0) & 0 & 0 & 0 \\ \partial f(x_0)/\partial x & f(x_0) & 0 & 0 \\ \partial f(x_0)/\partial x & 0 & f(x_0) & 0 \\ \partial^2 f(x_0)/\partial x^2 & \partial f(x_0)/\partial x & \partial f(x_0)/\partial x & f(x_0) \end{bmatrix}$$

$$\boxed{\begin{gathered} f(x_0) = f([x^*])_{11} \\ \partial f(x_0)/\partial x = f([x^*])_{21} = f([x^*])_{31} \\ \partial^2 f(x_0)/\partial x^2 = f([x^*])_{41} \end{gathered}}$$

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

- Compute the derivatives of $f(x) = x^2$ using the CR form for bidual numbers.

$$f(x) = x^{*2}$$

$$f(x^*) = \begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 1 & 0 & x_0 & 0 \\ 0 & 1 & 1 & x_0 \end{bmatrix}^2 = \begin{bmatrix} x_0^2 & 0 & 0 & 0 \\ 2x & x_0^2 & 0 & 0 \\ 2x & 0 & x_0^2 & 0 \\ 2 & 2x & 2x & x_0^2 \end{bmatrix}$$

$$f(x_0) = f([x^*])_{11} = x_0^2$$

$$\partial f(x_0)/\partial x = f([x^*])_{21} = 2x$$

$$\frac{\partial^2 f(x_0)}{\partial x^2} = f([x^*])_{41} = 2$$

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

- Compute the derivatives of $f(x) = x^3$ using the CR form for bidual numbers.

$$f(x) = x^{*3}$$

$$f(x^*) = \begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 1 & 0 & x_0 & 0 \\ 0 & 1 & 1 & x_0 \end{bmatrix}^3 = \begin{bmatrix} x_0^2 & 0 & 0 & 0 \\ 3x^2 & x_0^2 & 0 & 0 \\ 3x^2 & 0 & x_0^2 & 0 \\ 6x & 3x^2 & 3x^2 & x_0^2 \end{bmatrix}$$

$$f(x_0) = f([x^*])_{11} = x_0^2$$

$$\frac{\partial f(x_0)}{\partial x} = f([x^*])_{21} = 3x^2$$

$$\frac{\partial^2 f(x_0)}{\partial x^2} = f([x^*])_{41} = 6x$$

Closed-form example: $f(x) = e^x$

- Compute the derivatives of $f(x) = e^x$ using the CR form for bidual numbers.

$$f(x) = e^{x^*}$$

$$f(x^*) = \exp\left(\begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 1 & 0 & x_0 & 0 \\ 0 & 1 & 1 & x_0 \end{bmatrix}\right) = \begin{bmatrix} e^{x_0} & 0 & 0 & 0 \\ e^{x_0} & e^{x_0} & 0 & 0 \\ e^{x_0} & 0 & e^{x_0} & 0 \\ e^{x_0} & e^{x_0} & e^{x_0} & e^{x_0} \end{bmatrix}$$

$$f(x_0) = f([x^*])_{11} = e^{x_0}$$

$$\partial f(x_0)/\partial x = f([x^*])_{21} = e^{x_0}$$

$$\partial^2 f(x_0)/\partial x^2 = e^{x_0}$$

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

- Compute the derivatives of $f(x) = \cos(x)$using the CR form for bidual numbers.

$$f(x) = \sin(x^*)$$

$$f(x^*) = \sin\left(\begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 1 & 0 & x_0 & 0 \\ 0 & 1 & 1 & x_0 \end{bmatrix}\right) = \begin{bmatrix} \sin x_0 & 0 & 0 & 0 \\ \cos x_0 & \sin x_0 & 0 & 0 \\ \cos x_0 & 0 & \sin x_0 & 0 \\ -\sin x_0 & \cos x_0 & \cos x_0 & \sin x_0 \end{bmatrix}$$

$$f(x_0) = f([x^*])_{11} = \sin(x_0)$$

$$\frac{\partial f(x_0)}{\partial x} = f([x^*])_{21} = \cos(x_0)$$

$$\frac{\partial^2 f(x_0)}{\partial x^2} = -\sin(x_0)$$

Closed-form example: $f(x) = \cos(x)$

- Compute the derivatives of $f(x) = \cos(x)$using the CR form for bidual numbers.

$$f(x) = \cos(x^*)$$

$$f(x^*) = \cos\left(\begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 1 & 0 & x_0 & 0 \\ 0 & 1 & 1 & x_0 \end{bmatrix}\right) = \begin{bmatrix} \cos x_0 & 0 & 0 & 0 \\ -\sin x_0 & \cos x_0 & 0 & 0 \\ -\sin x_0 & 0 & \cos x_0 & 0 \\ -\cos x_0 & -\sin x_0 & -\sin x_0 & \cos x_0 \end{bmatrix}$$

$$f(x_0) = f([x^*])_{11} = \cos(x_0)$$

$$\frac{\partial f(x_0)}{\partial x} = f([x^*])_{21} = -\sin(x_0)$$

$$\frac{\partial^2 f(x_0)}{\partial x^2} = -\cos(x_0)$$

Closed-form example: $f(x) = \ln(x)$

- Compute the derivatives of $f(x) = \ln(x)$using the CR form for bidual numbers.

$$f(x) = \ln(x^*)$$

$$f(x^*) = \ln\left(\begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 1 & 0 & x_0 & 0 \\ 0 & 1 & 1 & x_0 \end{bmatrix}\right) = \begin{bmatrix} \ln(x_0) & 0 & 0 & 0 \\ 1/x_0 & \ln(x_0) & 0 & 0 \\ 1/x_0 & 0 & \ln(x_0) & 0 \\ -1/x_0^2 & 1/x_0 & 1/x_0 & \ln(x_0) \end{bmatrix}$$

$$f(x_0) = f([x^*])_{11} = \ln(x_0)$$

$$\frac{\partial f(x_0)}{\partial x} = f([x^*])_{21} = 1/x_0$$

$$\frac{\partial^2 f(x_0)}{\partial x^2} = -1/x_0^2$$

Computing derivatives using Bidual numbers using the CR form – general multivariate example

- To use bidual numbers to compute mixed derivatives, perturb x along ϵ_1 and y along ϵ_2, i.e.,

$$x^* = x_0 + h_1\epsilon_1 \qquad [x^*] = \begin{bmatrix} x_0 & 0 & 0 & 0 \\ h_1 & x_0 & 0 & 0 \\ 0 & 0 & x_0 & 0 \\ 0 & 0 & h_1 & x_0 \end{bmatrix}$$

$$y^* = y_0 + h_2\epsilon_2 \qquad [y^*] = \begin{bmatrix} y_0 & 0 & 0 & 0 \\ 0 & y_0 & 0 & 0 \\ h_2 & 0 & y_0 & 0 \\ 0 & h_2 & 0 & y_0 \end{bmatrix}$$

$$f([x^*, y^*]) = f\left(\begin{bmatrix} x_0 & 0 & 0 & 0 \\ h_1 & x_0 & 0 & 0 \\ 0 & 0 & x_0 & 0 \\ 0 & 0 & h_1 & x_0 \end{bmatrix}, \begin{bmatrix} y_0 & 0 & 0 & 0 \\ 0 & y_0 & 0 & 0 \\ h_2 & 0 & y_0 & 0 \\ 0 & h_2 & 0 & y_0 \end{bmatrix}\right) =$$

$$\begin{bmatrix} f(x_0) & 0 & 0 & 0 \\ h_1\partial f(x_0)/\partial x & f(x_0) & 0 & 0 \\ h_2\partial f(x_0)/\partial x & 0 & f(x_0) & 0 \\ h_1h_2\partial^2 f(x_0)/\partial x\partial y & h_2\partial f(x_0)/\partial x & h_1\partial f(x_0)/\partial x & f(x_0) \end{bmatrix}$$

$$f(x_0) = f([x^*])_{11}$$

$$\frac{\partial f(x_0)}{\partial x} = \frac{1}{h_1} f([x^*],[y^*])_{21}$$

$$\frac{\partial f(x_0)}{\partial y} = \frac{1}{h_2} f([x^*],[y^*])_{31}$$

$$\frac{\partial^2 f(x_0)}{\partial x\partial y} = \frac{1}{h_1h_2} f([x^*])_{41}$$

Computing derivatives using Bidual numbers using the CR form – recommended <u>multivariate</u> example

- The recommendation is to use $h_1 = h_2 = 1$.

$$x^* = x + h_1\epsilon_1 \qquad [x^*] = \begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 0 & 0 & x_0 & 0 \\ 0 & 0 & 1 & x_0 \end{bmatrix} \qquad y^* = y + h_2\epsilon_2 \quad [y^*] = \begin{bmatrix} y_0 & 0 & 0 & 0 \\ 0 & y_0 & 0 & 0 \\ 1 & 0 & y_0 & 0 \\ 0 & 1 & 0 & y_0 \end{bmatrix}$$

$$f([x^*, y^*]) = f\left(\begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 0 & 0 & x_0 & 0 \\ 0 & 0 & 1 & x_0 \end{bmatrix}, \begin{bmatrix} y_0 & 0 & 0 & 0 \\ 0 & y_0 & 0 & 0 \\ 1 & 0 & y_0 & 0 \\ 0 & 1 & 0 & y_0 \end{bmatrix}\right) =$$

$$\begin{bmatrix} f(x_0) & 0 & 0 & 0 \\ \partial f(x_0)/\partial x & f(x_0) & 0 & 0 \\ \partial f(x_0)/\partial y & 0 & f(x_0) & 0 \\ \partial^2 f(x_0)/\partial x^2 & \partial f(x_0)/\partial y & \partial f(x_0)/\partial x & f(x_0) \end{bmatrix}$$

$$\boxed{\begin{gathered} f(x_0) = f([x^*])_{11} \\ \frac{\partial f(x_0)}{\partial x} = f([x^*],[y^*])_{21} \\ \frac{\partial f(x_0)}{\partial y} = f([x^*],[y^*])_{31} \\ \frac{\partial^2 f(x_0)}{\partial x \partial y} = f([x^*])_{41} \end{gathered}}$$

Closed-form example: $f(x) = xy$

- Compute the derivatives of $f(x) = xy$ using the CR form for bidual numbers.

$$x^* = x_0 + h_1\epsilon_1 \qquad [x^*] = \begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 0 & 0 & x_0 & 0 \\ 0 & 0 & 1 & x_0 \end{bmatrix} \qquad y^* = y_0 + h_2\epsilon_2 \qquad [y^*] = \begin{bmatrix} y_0 & 0 & 0 & 0 \\ 0 & y_0 & 0 & 0 \\ 1 & 0 & y_0 & 0 \\ 0 & 1 & 0 & y_0 \end{bmatrix}$$

$$f(x) = x^* y^*$$

$$f(x^*) = \begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 0 & 0 & x_0 & 0 \\ 0 & 0 & 1 & x_0 \end{bmatrix} \begin{bmatrix} y_0 & 0 & 0 & 0 \\ 0 & y_0 & 0 & 0 \\ 1 & 0 & y_0 & 0 \\ 0 & 1 & 0 & y_0 \end{bmatrix} = \begin{bmatrix} x_0^2 y_0^2 & 0 & 0 & 0 \\ 2x_0 y_0^2 & x_0^2 y_0^2 & 0 & 0 \\ 2x_0^2 y_0 & 0 & x_0^2 y_0^2 & 0 \\ 4x_0 y_0 & 2x_0^2 y_0 & 2x_0 y_0^2 & x_0^2 y_0^2 \end{bmatrix}$$

$$f(x_0, y_0) = f([x^* y^*])_{11} = x_0 y_0$$

$$\frac{\partial f(x_0, y_0)}{\partial x} = f([x^*, y^*])_{21} = 2x_0 y_0^2; \quad \frac{\partial f(x_0, y_0)}{\partial y} = f([x^*, y^*])_{31} = 2x_0^2 y_0$$

$$\frac{\partial^2 f(x_0)}{\partial x^2} = 4x_0 y_0$$

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

- Compute the derivatives of $f(x) = x^2y^2$ using the CR form for bidual numbers.

$$x^* = x_0 + h_1\epsilon_1 \qquad [x^*] = \begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 0 & 0 & x_0 & 0 \\ 0 & 0 & 1 & x_0 \end{bmatrix} \qquad y^* = y_0 + h_2\epsilon_2 \qquad [y^*] = \begin{bmatrix} y_0 & 0 & 0 & 0 \\ 0 & y_0 & 0 & 0 \\ 1 & 0 & y_0 & 0 \\ 0 & 1 & 0 & y_0 \end{bmatrix}$$

$$f(x) = {x^*}^2{y^*}^2$$

$$f(x^*) = \begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 1 & 0 & x_0 & 0 \\ 0 & 1 & 1 & x_0 \end{bmatrix}^2 \begin{bmatrix} y_0 & 0 & 0 & 0 \\ 0 & y_0 & 0 & 0 \\ 1 & 0 & y_0 & 0 \\ 0 & 1 & 0 & y_0 \end{bmatrix}^2 = \begin{bmatrix} x_0^2y_0^2 & 0 & 0 & 0 \\ 2x_0y_0^2 & x_0^2y_0^2 & 0 & 0 \\ 2x_0^2y_0 & 0 & x_0^2y_0^2 & 0 \\ 4x_0y_0 & 2x_0^2y_0 & 2x_0y_0^2 & x_0^2y_0^2 \end{bmatrix}$$

$$f(x_0, y_0) = f([x^*y^*])_{11} = x_0y_0$$

$$\frac{\partial f(x_0, y_0)}{\partial x} = f([x^*, y^*])_{21} = 2x_0y_0^2; \qquad \frac{\partial f(x_0, y_0)}{\partial y} = f([x^*, y^*])_{31} = 2x_0^2y_0$$

$$\frac{\partial^2 f(x_0)}{\partial x^2} = 4x_0y_0$$

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

- Compute the derivatives of $f(x) = x \sin y$ using the CR form for bidual numbers.

$$x^* = x_0 + h_1\epsilon_1 \qquad [x^*] = \begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 0 & 0 & x_0 & 0 \\ 0 & 0 & 1 & x_0 \end{bmatrix} \qquad y^* = y_0 + h_2\epsilon_2 \qquad [y^*] = \begin{bmatrix} y_0 & 0 & 0 & 0 \\ 0 & y_0 & 0 & 0 \\ 1 & 0 & y_0 & 0 \\ 0 & 1 & 0 & y_0 \end{bmatrix}$$

$$f(x) = x^* \sin y^*$$

$$f(x^*) = \begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 0 & 0 & x_0 & 0 \\ 0 & 0 & 1 & x_0 \end{bmatrix} \sin\left(\begin{bmatrix} y_0 & 0 & 0 & 0 \\ 0 & y_0 & 0 & 0 \\ 1 & 0 & y_0 & 0 \\ 0 & 1 & 0 & y_0 \end{bmatrix}\right) = \begin{bmatrix} x_0 \sin(y_0) & 0 & 0 & 0 \\ \sin(y_0) & x_0 \sin(y_0) & 0 & 0 \\ x_0 \sin(y_0) & 0 & x_0 \sin(y_0) & 0 \\ \cos(y_0) & x_0 \sin(y_0) & \sin(y_0) & x_0 \sin(y_0) \end{bmatrix}$$

$$\boxed{\begin{gathered} f(x_0, y_0) = f([x^* y^*])_{11} = x_0 y_0 \\ \frac{\partial f(x_0, y_0)}{\partial x} = f([x^*, y^*])_{21} = \sin(y_0)\,; \quad \frac{\partial f(x_0, y_0)}{\partial y} = f([x^*, y^*])_{31} = x_0 \sin(y_0) \\ \frac{\partial^2 f(x_0)}{\partial x^2} = \cos(y_0) \end{gathered}}$$

Closed-form example: $f(x) = xe^y$

- Compute the derivatives of $f(x) = xe^x$ using the CR form for bidual numbers.

$$x^* = x_0 + h_1\epsilon_1 \qquad [x^*] = \begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 0 & 0 & x_0 & 0 \\ 0 & 0 & 1 & x_0 \end{bmatrix} \qquad y^* = y_0 + h_2\epsilon_2 \qquad [y^*] = \begin{bmatrix} y_0 & 0 & 0 & 0 \\ 0 & y_0 & 0 & 0 \\ 1 & 0 & y_0 & 0 \\ 0 & 1 & 0 & y_0 \end{bmatrix}$$

$$f(x) = xe^x$$

$$f(x^*) = \begin{bmatrix} x_0 & 0 & 0 & 0 \\ 1 & x_0 & 0 & 0 \\ 0 & 0 & x_0 & 0 \\ 0 & 0 & 1 & x_0 \end{bmatrix} \exp\left[\begin{bmatrix} y_0 & 0 & 0 & 0 \\ 0 & y_0 & 0 & 0 \\ 1 & 0 & y_0 & 0 \\ 0 & 1 & 0 & y_0 \end{bmatrix}\right] = \begin{bmatrix} x_0^2y_0^2 & 0 & 0 & 0 \\ 2x_0y_0^2 & x_0^2y_0^2 & 0 & 0 \\ 2x_0^2y_0 & 0 & x_0^2y_0^2 & 0 \\ 4x_0y_0 & 2x_0^2y_0 & 2x_0y_0^2 & x_0^2y_0^2 \end{bmatrix}$$

$$f(x_0, y_0) = f([x^*y^*])_{11} = x_0y_0$$

$$\frac{\partial f(x_0, y_0)}{\partial x} = f([x^*, y^*])_{21} = 2x_0y_0^2; \quad \frac{\partial f(x_0, y_0)}{\partial y} = f([x^*, y^*])_{31} = 2x_0^2y_0$$

$$\frac{\partial^2 f(x_0)}{\partial x^2} = 4x_0y_0$$

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