Derivation of dual numbers for first order sensitivities

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Dual numbers for first order sensitivities

- Dual numbers can also be used to compute highly accuracy first order sensitivities. A comparison between Complex and Dual numbers is shown below.

	Complex	**Dual**
Format	$a + bi$	$a + b\epsilon$
Real part	a	a
Imaginary part	b	b
Imaginary unit	i	ϵ
Imaginary unit squared	$i^2 = -1$	$\epsilon^2 = 0, \epsilon \neq 0$
$f'(x)$	$Im(f(x + ih))/h$	$Im(f(x + h\epsilon))/h$
Step size h	$10^{-8} < h < 10^{-308}$	Arbitrary, typically $h = 1$
Cauchy-Reimann matrix - general	$\begin{pmatrix} a & -b \\ b & a \end{pmatrix}$	$\begin{pmatrix} a & 0 \\ b & a \end{pmatrix}$
Cauchy-Reimann matrix - differentiation	$\begin{pmatrix} x & -h \\ h & x \end{pmatrix}$	$\begin{pmatrix} x & 0 \\ 1 & x \end{pmatrix}$
Type	Numerical	Symbolic or Numerical

Dual number definition

- A dual number is analogous to a complex number in that it contains a real and an imaginary part.
  - $x^* = a + b\epsilon$
  - With $\epsilon^2 = 0, \quad \epsilon \neq 0$
- Dual numbers are well known for automatic differentiation; however, they are not built into programming languages although there are often packages that can be used.
- In our case, we will use MultiZ to define and operate with dual numbers.

```
from multiZ.symdual import *
a,b = sym.Symbol('a'),sym.Symbol('b')
x = sdual(a, b)

print(x)
#Output sdual(a, b): Represents a symbolic dual number of the form x = a + bε
```

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Dual number – basic operations

$a, b, r - real\ \ numbers$

- Addition/subtraction
  - $(a + b\epsilon) \pm (c + d\epsilon) = (a \pm c) + (b \pm d)\epsilon$

- Multiplication of 2 dual numbers
  - $(a + b\epsilon)(c + d\epsilon) = ac + ad\epsilon + bc\epsilon + bd\cancelto{0}{\epsilon^2}$
  - $ac + (ad + bc)\epsilon$

- Multiplication of a real times a dual number
  - $(r)(a + b\epsilon) = (ra + rb\epsilon)$

- Multiplication of a pure dual number times a dual number
  - $(\epsilon)(a + b\epsilon) = a\epsilon$

Dual numbers - division

- Division of two dual numbers
  - $\frac{a+b\epsilon}{c+d\epsilon} = \frac{a+b\epsilon}{c+d\epsilon}\frac{c-d\epsilon}{c-d\epsilon} = \frac{ac+(bc-ad)\epsilon}{c^2} = \frac{a}{c} + \left(\frac{bc-ad}{c^2}\right)\epsilon$
- Division of a dual number by a real number
  - $\frac{a+b\epsilon}{r} = \frac{a}{r} + \left(\frac{b}{r}\right)\epsilon$
- Division of a real number by a dual number
  - $\frac{r}{a+b\epsilon} = \frac{r}{a+b\epsilon}\frac{a-b\epsilon}{a-b\epsilon} = \frac{ra-rb\epsilon}{a^2} = \frac{r}{a} + \left(\frac{-rb}{a^2}\right)\epsilon$

- Note, division by a dual number of the form $(0+\epsilon)$ is not defined.

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Functions of dual numbers

- Functions of dual numbers can be determined in a straightforward manner using the Taylor series definition of a dual number. This definition is,
  - $f(a + b\epsilon) = f(a) + b\frac{df}{dx}(a)\epsilon$
- Note, the function f and its derivative are only evaluated at the real number a.

Function	Mathematical expression
$\sin(a + b\epsilon)$	$\sin(a) + b\cos(a)\,\epsilon$
$\cos(a + b\epsilon)$	$\cos(a) - b\sin(a)\,\epsilon$
$\cosh(a + b\epsilon)$	$\cosh(a) + b\sinh(a)\,\epsilon$
$\sqrt{a + b\epsilon}$	$\sqrt{a} + \frac{b}{2\sqrt{a}}\epsilon$
$\ln(a + b\epsilon)$	$\ln(a) + \frac{b}{a}\epsilon$
$e^{a+b\epsilon}$	$e^{a} + be^{a}\epsilon$
$\sin(a + b\epsilon)^{-1}$	$\sin^{-1}(a) + \frac{b}{\sqrt{1 - a^2}}$

Dual number raised to a dual power

- Use the mathematical expression $x^y = e^{y\ln(x)}$
  - $(a+b\epsilon)^{c+d\epsilon} = e^{(c+d\epsilon)\ln(a+b\epsilon)}$
  - Substituting: $\ln(a+b\epsilon) = \ln(a) + \left(\frac{b}{a}\right)\epsilon$ we obtain
  - $(a+b\epsilon)^{c+d\epsilon} = a^c + a^{c-1}(ad\ ln(a) + cb)\epsilon$
- Real raised to a dual power – this is a subset of the above equation with $\mathrm{a} = \mathrm{r}$ and $b = 0$.
  - $(\mathrm{r})^{c+d\epsilon} = r^c + r^c\left(rd\ ln(r)\right)\epsilon$
- Dual raised to a real power - this is a subset of the above equation with $c = n$ and $d = 0$.
  - $(a+b\epsilon)^n = a^n + a^{n-1}nb\epsilon$

Dual Numbers for first order sensitivities

- Dual numbers can be used to compute highly accuracy first order sensitivities. Consider the Taylor series expansion of a dual number $a + b\varepsilon$ expanded about a

$$f(a+b\epsilon) \approx f(a) + \frac{df}{dx}(a)b\epsilon + \frac{1}{2}\frac{d^2f}{dx^2}(a)\cancelto{0}{(b\epsilon)^2} + \frac{1}{3!}\frac{d^3f}{dx^3}(a)\cancelto{0}{(b\epsilon)^3} + \cancelto{0}{HOT}$$

Using the fact that $\epsilon^n = 0$ for $n \geq 2$, we obtain,

$$f(a+b\epsilon) = f(a) + \frac{df}{dx}(a)b\epsilon$$

$$f'(a) = \frac{1}{h}Im(f(a+h\epsilon))$$

h is arbitrary so $h = 1$ is typically used. In this case

$$\boxed{\frac{df}{dx}(a) = Im(f(a+\epsilon))}$$

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