Computing derivatives using bidual numbers – univariate example

- Consider a Taylor series expansion of the following bidual number

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

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

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

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: $h_1 = h_2 = 1$

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

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

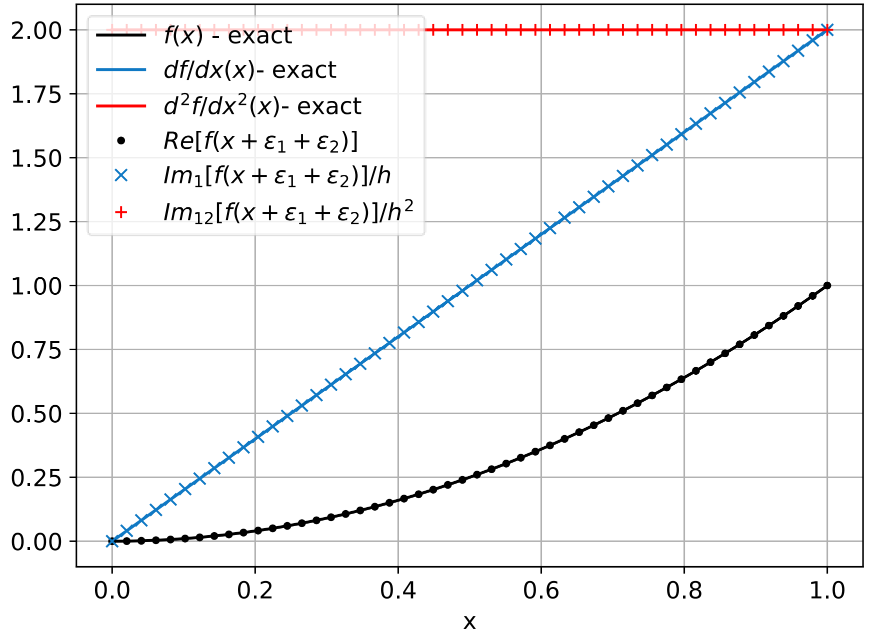
$$\frac{d^2 f}{dx^2} = Im_{12}(f(x^*))$$

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 $h_1 = h_2 = 1$.

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

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



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 $h_1 = h_2 = 1$.

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

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

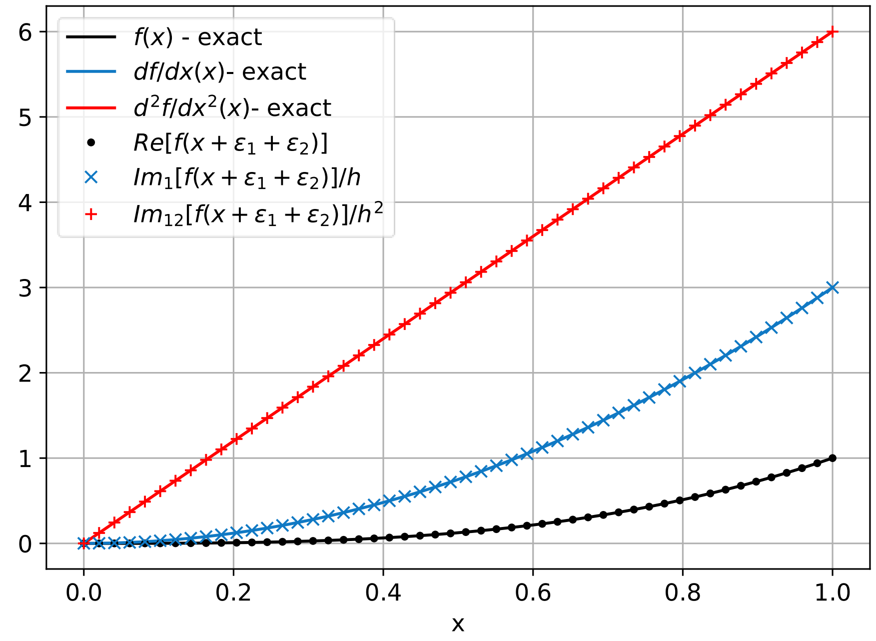
$$x^3 + 3x^2\epsilon_1 + 3x^2\epsilon_2 + 6x\epsilon_1\epsilon_2 + 3x\cancel{\epsilon_1^2}^{0} + 3x\cancel{\epsilon_2^2}^{0} + 3\epsilon_1\cancel{\epsilon_2^2}^{0} + 3\cancel{\epsilon_1^2}^{0}\epsilon_2 + \cancel{\epsilon_1^3}^{0} + \cancel{\epsilon_2^3}^{0}$$

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

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

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

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

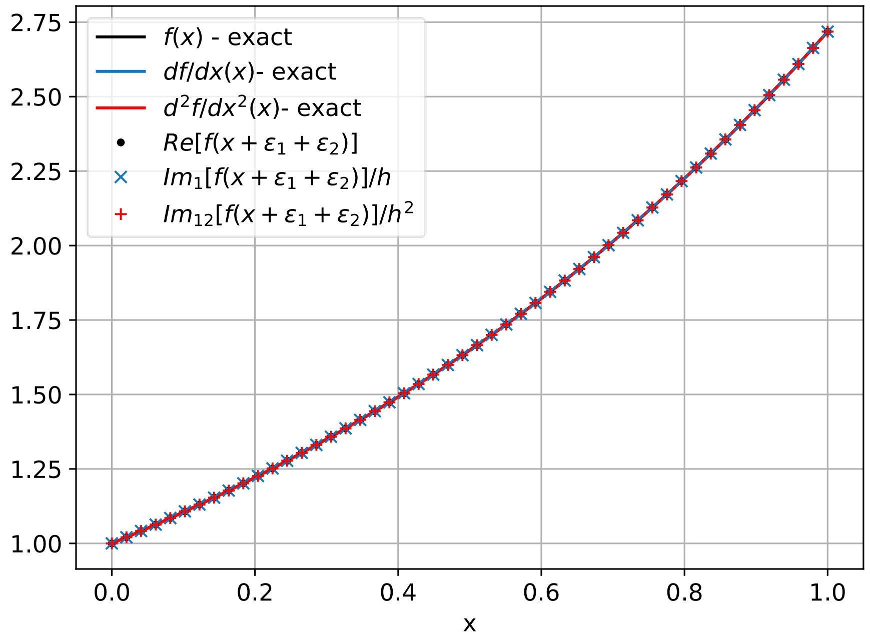


Closed-form example: $f(x) = e^x$

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

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

$$\frac{df}{dx} = Im_1\big(f(x + \epsilon_1 + \epsilon_2)\big) = Im_2\big(f(x + \epsilon_1 + \epsilon_2)\big)$$
$$= Im_1(e^{x+\epsilon_1+\epsilon_2}) = e^x$$
$$\frac{d^2f}{dx^2} = Im_{12}\big(f(x + \epsilon)\big) = Im_{12}(e^{x+\epsilon_1+\epsilon_2}) = e^x$$

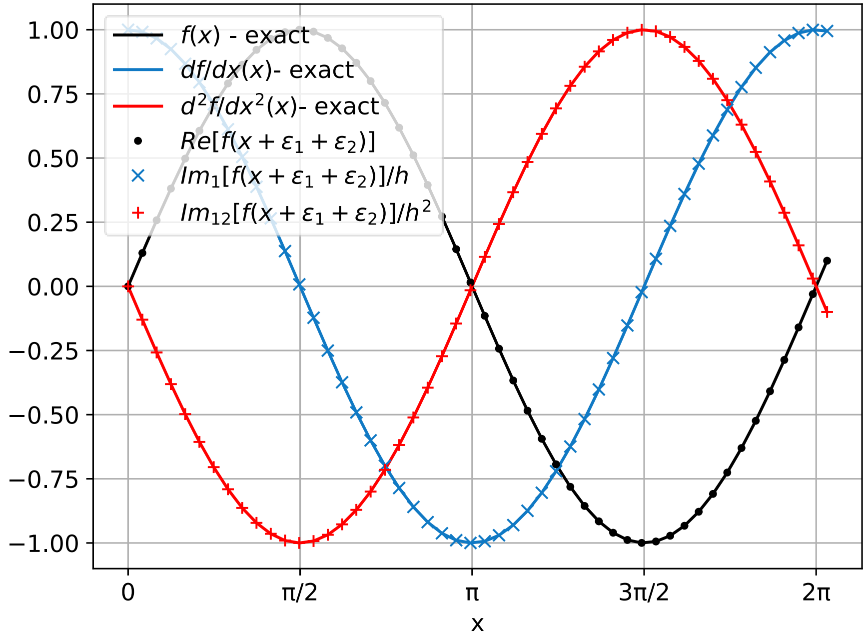


Closed-form example: $f(x) = \sin(x)$

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

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

$$\frac{df}{dx} = Im_1\big(f(x+\epsilon)\big) = Im_2\big(f(x+\epsilon)\big) = Im_1(\sin(x+\epsilon_1+\epsilon_2))$$
$$= \cos(x)$$
$$\frac{d^2f}{dx^2} = Im_{12}\big(f(x+\epsilon)\big) = Im_{12}(\sin(x+\epsilon_1+\epsilon_2)) = -\sin(x)$$

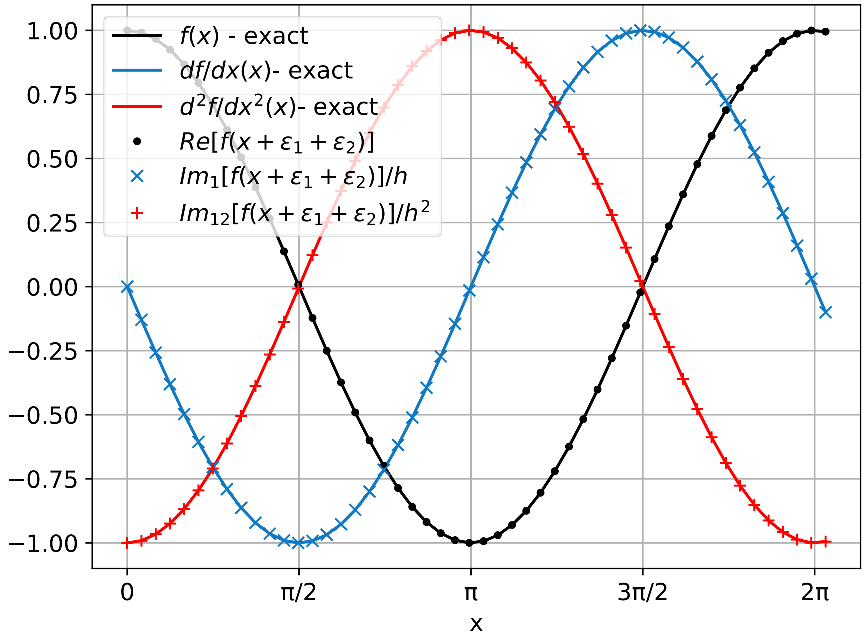


Closed-form example: $f(x) = \cos(x)$

- 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 $h_1 = h_2 = 1$.

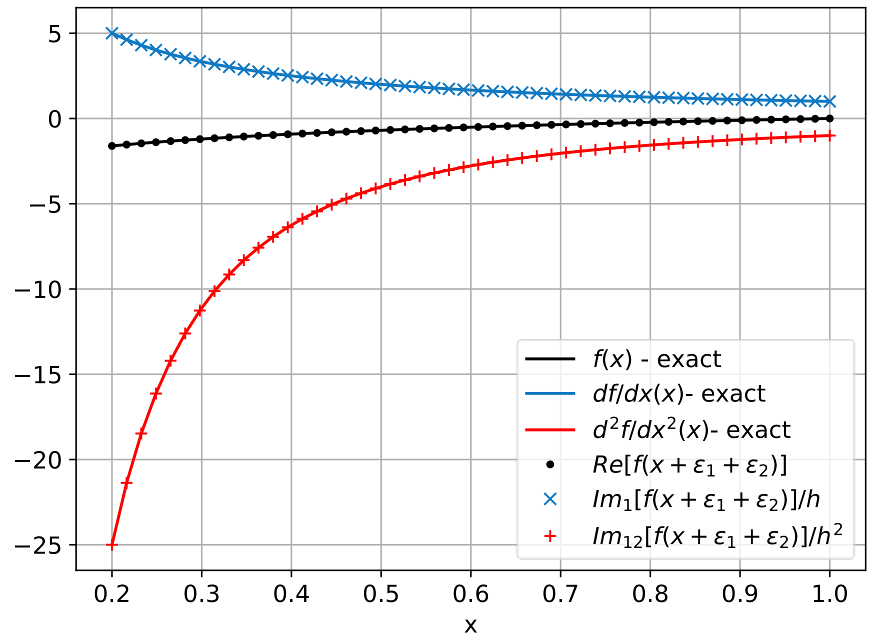
$$f(x) = \ln(x)$$

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

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

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

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



Computing derivatives using bidual numbers – multivariate example

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

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

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

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

General Case: arbitrary h

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

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

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Computing derivatives using bidual numbers – multivariate example

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

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

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

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

Recommended: $h = 1$

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

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

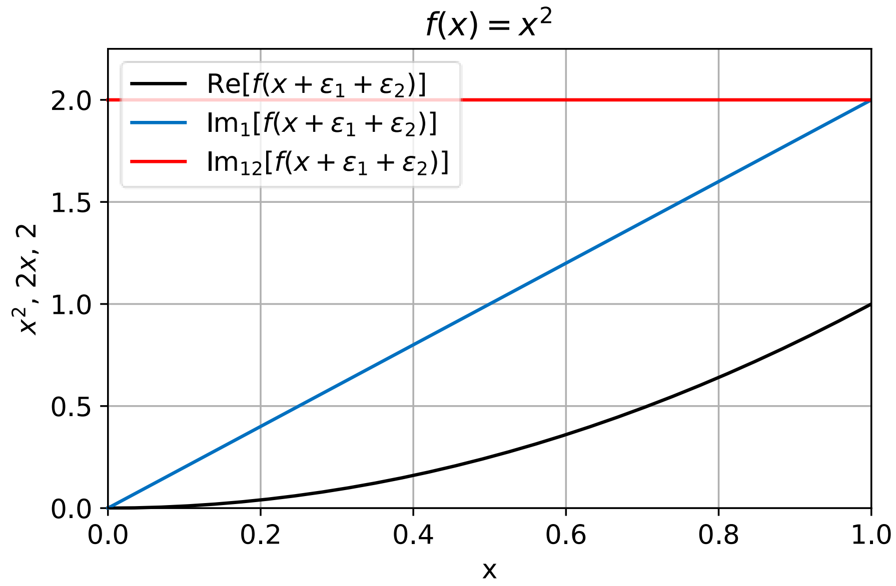
Closed-form example: $f(x,y) = xy$

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

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

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

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

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

$$f(x, y) = x\,e^y$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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Incorrect method for computing derivatives using bidual numbers – univariate example

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

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

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

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

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

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

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

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