Computational Physics
PHZ4151C

Numerical Derivatives

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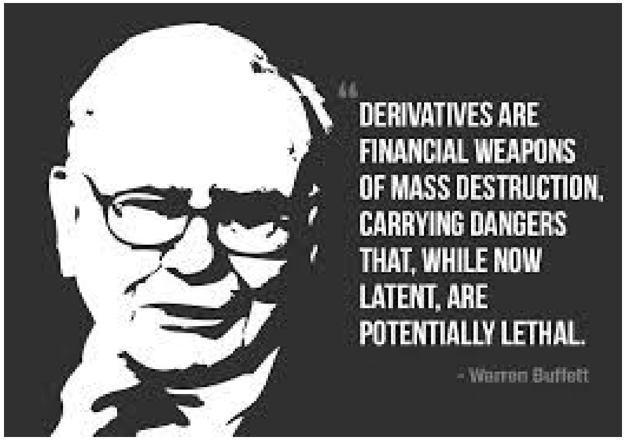

Numerical Differentiation

READ Discussions in

Chapter 5.10

Numerical Differentiation

- Often possible to find derivatives given an analytic expression for a function
- But this is not always the case. In some cases, numerical determination of the derivative is the only alternative
  - Functions available only as a set of discrete data points
  - Determination of a function from non-linear differential equation and some initial conditions
- But there are some significant practical problems with numerical derivatives...

Simple Derivatives

Limit-based determination: $$\frac{df(x)}{dx} = lim_{h \to 0} \left[\frac{f(x+h) - f(x)}{h} \right]$$

Another method of computing differences:

Forward Difference

$$D_h^+(f(x)) = \left[\frac{f(x+h) - f(x)}{h} \right]$$

Backward Difference

$$D_h^-(f(x)) = \left[\frac{f(x) - f(x-h)}{h} \right]$$

Forward and backward differences typically give about the same result with similar accuracy

Only a few special cases where one is preferred

- at a discontinuity
- at the boundary of bounded functions

Derivatives & Errors

$O(h^2)$

remaining term

Taylor Series Expansion:

$$f(x+h) = f(x) + h\frac{d\,f(x)}{dx} + \frac{h^2}{2}\frac{d^2 f(x)}{dx^2} + \ldots$$

Forward Difference

$$\left[\frac{f(x+h) - f(x)}{h}\right] = \frac{d\,f(x)}{dx} + O(h)$$

approximation error

$$\epsilon_a = \frac{h}{2}\left|f''(x)\right|$$

This implies that making *h* smaller, reduces the total error (Not TRUE)

Why?.......

Derivatives & Errors

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This implies that making *h* smaller, reduces the total error (Not TRUE)

Why?....... Round-off errors!

Forward Difference Error

$$\epsilon = \epsilon_c + \epsilon_a$$

round-off error

$$\epsilon_c = \frac{2c\, f(x)}{h}$$

approximation error

$$\epsilon_a = \frac{h}{2} |f''(x)|$$

$$\epsilon = \frac{2c|f(x)|}{h} + \frac{1}{2} h |f''(x)|$$

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recall from numerical accuracy

$$x_c = x_{true}(1 \pm c)$$

$$f_c(x) = f(x) \pm c\, f(x)$$

$$D^+[f(x)] = \frac{f(x+h) - f(x)}{h} \pm \frac{2c\, f(x)}{h}$$

Forward Difference Error

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round-off error

$$\epsilon_c = \frac{2c\, f(x)}{h}$$

approximation error

$$\epsilon_a = \frac{h}{2}|f''(x)|$$

$$\epsilon = \frac{2c|f(x)|}{h} + \frac{1}{2}h|f''(x)|$$

setting $\frac{d\epsilon}{dh} = 0$ to find the value of h which minimizes the error

$$h_{best} = \sqrt{4c\left|\frac{f(x)}{f''(x)}\right|}$$

recall from numerical accuracy

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setting $\frac{d\epsilon}{dh} = 0$ to find the value of h which minimizes the error

$$h_{best} = \sqrt{4c\left|\frac{f(x)}{f''(x)}\right|}$$

$$\boxed{\epsilon = h|f''(x)| = \sqrt{4c|f(x)\, f''(x)|}}$$

recall from numerical accuracy

$$x_c = x_{true}(1 \pm c)$$

$$f_c(x) = f(x) \pm c\, f(x)$$

$$D^+[f(x)] = \frac{f(x+h) - f(x)}{h} \pm \frac{2c\, f(x)}{h}$$

if f(x) & f''(x) are on the order 1,
we should choose a h on the order $\sqrt{c}$
which is typically 10^{-8} for 64bit operations

Central Difference

Limit-based determination:

$$\frac{df(x)}{dx} = \lim_{h \to 0} \left[\frac{f(x+h) - f(x)}{h} \right]$$

Another method of computing differences:

Central Difference

$$D_h^c(f(x)) = \left[\frac{f(x+h/2) - f(x-h/2)}{h} \right]$$

The Central Difference is overall more accurate

Central Difference Error

Taylor expansion:

$$f(x+h/2)=f(x)+(h/2)f'(x)+\frac{(h/2)^2}{2}f''(x)+\frac{(h/2)^3}{6}f'''(x)+\ldots$$

$$-\quad f(x-h/2)=f(x)+(-h/2)f'(x)+\frac{(h/2)^2}{2}f''(x)+\frac{(-h/2)^3}{6}f'''(x)+\ldots$$

$$f(x+h/2)-f(x-h/2) \quad = \quad h f'(x)+\frac{h^3}{24}f'''(x)+\ldots$$

Central Difference Error

Taylor expansion:

$$f(x+h/2) = f(x) + (h/2)f'(x) + \frac{(h/2)^2}{2} f''(x) + \frac{(h/2)^3}{6} f'''(x) + \ldots$$

$$- \quad f(x-h/2) = f(x) + (-h/2)f'(x) + \frac{(h/2)^2}{2} f''(x) + \frac{(-h/2)^3}{6} f'''(x) + \ldots$$

$$f(x+h/2) - f(x-h/2) = h f'(x) + \frac{h^3}{24} f'''(x) + \ldots$$

Central Difference

$$\left[\frac{f(x+h/2) - f(x-h/2)}{h}\right] = \frac{d f(x)}{dx} + O(h^2)$$

truncation error term is of order in h^2

Central Difference Error

$$\epsilon = \epsilon_c + \epsilon_a$$

round-off error

$$\epsilon_c = \frac{2c\, f(x)}{h}$$

approximation error

$$\epsilon_a = \frac{h^2}{24} |f'''(x)|$$

$$\epsilon = \frac{2c|f(x)|}{h} + \frac{1}{24} h^2 |f'''(x)|$$

Central Difference Error

$$\epsilon = \epsilon_c + \epsilon_a$$

round-off error

$$\epsilon_c = \frac{2c\, f(x)}{h}$$

approximation error

$$\epsilon_a = \frac{h^2}{24}|f'''(x)|$$

$$\epsilon = \frac{2c|f(x)|}{h} + \frac{1}{24}h^2|f'''(x)|$$

setting $\frac{d\epsilon}{dh} = 0$ to find the value of h which minimizes the error

$$h_{best} = \left(24c\left|\frac{f(x)}{f'''(x)}\right|\right)^{1/3}$$

$$\boxed{\epsilon = \frac{1}{8}h^2|f'''(x)| = \left(24c|f(x)\,f'''(x)|\right)^{1/3}}$$

if f(x) & f '''(x) are on the order 1, we should choose a *h* on the order of 10^{-5}
but the error will be on the order of 10^{-10}

Central Difference Example

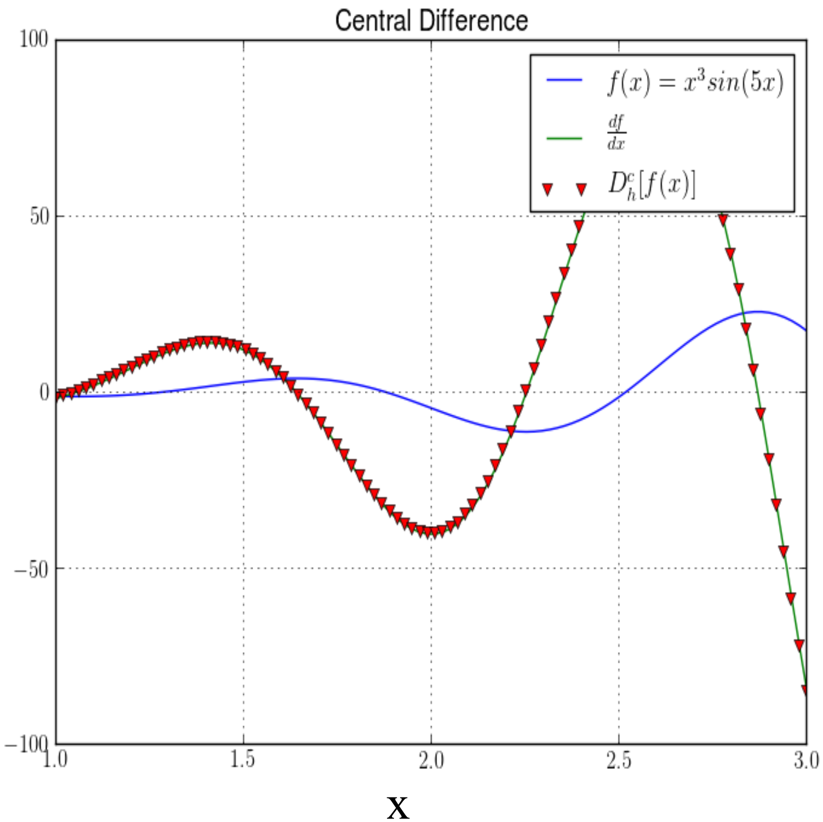
$$f(x) = x^3 \sin(5x)$$

$$D_h^c[f(x)] = \frac{d\,f(x)}{dx} + O(h^2)$$

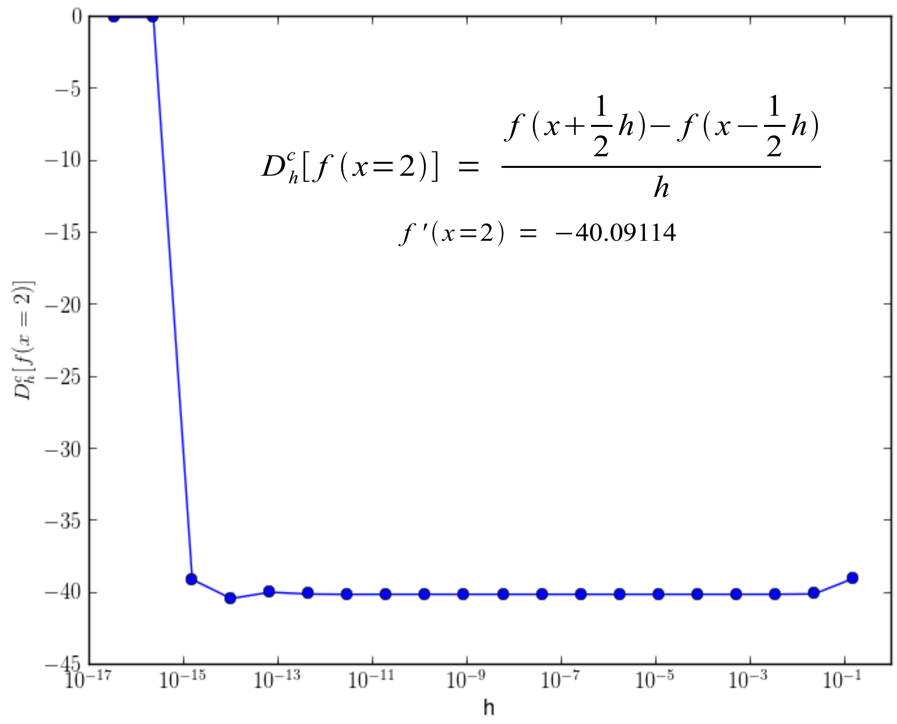
```
def F(x):
    return x**3 * np.sin(5*x)

def dFdx_numerical(func, x, h=1e-5):
    """ Numerical derivative using Central Difference """
    return (func(x+0.5*h) - func(x-0.5*h)) / h


def dFdx(x):
    """ Analytic derivative """
    return  3*x**2 * np.sin(5*x) + 5*x**3 * cos(5*x)
```



centralDiff.py



$$f'(x) = 3x^2 \sin(5x) + 5x^3 \cos(5x)$$

Second Derivatives

calculate by applying the first-derivative formulas twice

$$f'(x+h/2) \simeq \frac{f(x+h)-f(x)}{h} \qquad f'(x-h/2) \simeq \frac{f(x)-f(x-h)}{h}$$

Second Derivatives

calculate by applying the first-derivative formulas twice

$$f'(x+h/2) \simeq \frac{f(x+h)-f(x)}{h} \qquad f'(x-h/2) \simeq \frac{f(x)-f(x-h)}{h}$$

The central difference for the second-derivative:

$$f''(x) \simeq \frac{f'(x+h/2)-f'(x-h/2)}{h}$$

$$= \frac{[f(x+h)-f(x)]/h-[f(x)-f(x-h)]/h}{h}$$

2nd Central Difference

$$\boxed{= \frac{f(x+h)-2\mathrm{f}(x)+f(x-h)}{h^2}}$$

2^{nd} Central Difference Error

From the Taylor expansion:

$$f(x+h)=f(x)+h\,f'(x)+\frac{1}{2}h^2 f''(x)+\frac{1}{6}h^3 f'''(x)+\frac{1}{24}f''''(x)+\ldots$$

$$+\quad f(x-h)=f(x)-h\,f'(x)+\frac{1}{2}h^2 f''(x)-\frac{1}{6}h^3 f'''(x)+\frac{1}{24}f''''(x)+\ldots$$

$$f(x+\Delta x/2)-f(x-\Delta x/2) \;=\; \Delta x\, f'(x)+\frac{\Delta x^3}{24}f'''(x)+\ldots$$

2^{nd} Central Difference

$$\left[\frac{f(x+h)-2\mathrm{f}(x)+f(x-h)}{h^2}\right] = f''(x) - \frac{1}{12}h^2 f''''(x) + \ldots$$

truncation error term is
of order in h^2

2^{nd} Central Difference Error

$$\epsilon = \epsilon_c + \epsilon_a$$

round-off error

$$\epsilon_c = \frac{4c\, f(x)}{h^2}$$

approximation error

$$\epsilon_a = \frac{h^2}{12} |f''''(x)|$$

$$\epsilon = \frac{4c|f(x)|}{h^2} + \frac{1}{12} h^2 |f''''(x)|$$

setting $\frac{d\epsilon}{dh} = 0$ to find the value of h which minimizes the error

$$h_{best} = \left(48c \left| \frac{f(x)}{f''''(x)} \right| \right)^{1/4}$$

$$\boxed{\epsilon = \frac{1}{6} h^2 |f''''(x)| = \left(\frac{4}{3} c |f(x) f''''(x)| \right)^{1/2}}$$

if f(x) & f ''''(x) are on the order 1, for an error on the order of 10^{-8} one should choose h to be on the order of 10^{-4}

This Week's exercise

Radioactive Decays

$$\frac{dN(t)}{dt} = \frac{-N(t)}{\tau}$$

$$Set\ \frac{dN(t)}{dt} = D_h^+(N(t)) = \frac{N(t+h) - N(t)}{h}$$

and solve for the incremental equation

$$\frac{N(t+h) - N(t)}{h} = -\frac{N(t)}{\tau}$$

$$N(t+h) = N(t) - \frac{h}{\tau} N(t)$$

initial conditions
at t(0):
N(t=0) = 100%

$$N_{i+1} = N_i \left(1 - \frac{h}{\tau} \right)$$

incremental equation

Let's get working