Numerical Differentiation

motivation

- sections on numerical differentiation and integration mirror core topics of calculus
- approximations of derivatives used in
    - solution of nonlinear equations
    - solution of ordinary and partial differential equations
    - data analysis
- determination of derivatives from measured data is archetypical example of an *ill-posed problem*
- problem: determine $f'(x)$ from finite number of values $f(x_i)$ which may contain errors
- use definition from calculus as a guide:

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

- approach: take derivative of interpolating polynomial

truncation error

- Taylor expansion

$$\frac{f(x+h)-f(x)}{h} = \frac{[f(x)+hf'(x)+f''(\xi)h^2/2]-f(x)}{h}$$
$$= f'(x) + \frac{f''(\xi)}{2}h$$

for some $\xi \in [x, x+h]$

- for bounded f'' and $h \to 0$

$$e_h(x) := f'(x) - \frac{f(x+h)-f(x)}{h} = O(h) \to 0$$

this is the *truncation error*

- also: consider rounding error!

example $f(x) = x\sin(x)$ for $x = 1$

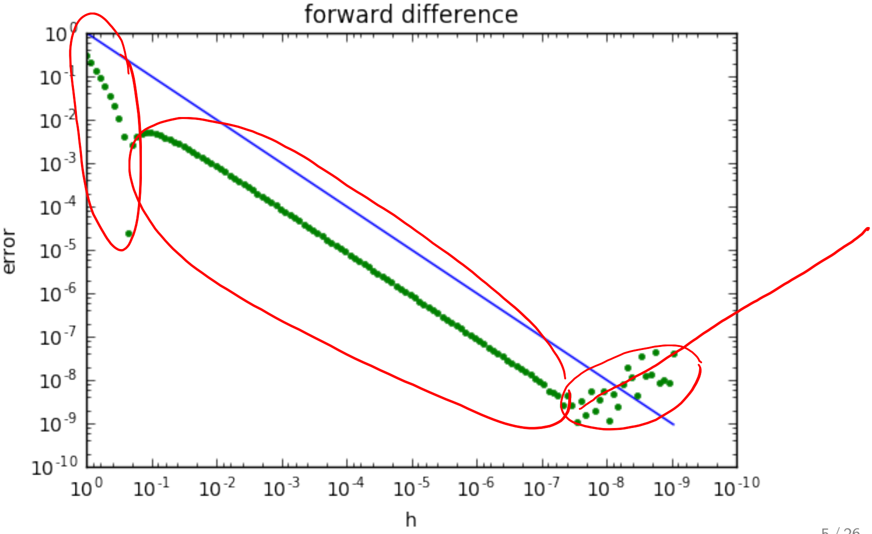
- exact derivative $f'(x) = \sin(x) + x\cos(x)$
- rel. error

$$e_h = \left| \frac{\frac{f(x+h)-f(x)}{h} - f'(x)}{f'(x)} \right|$$

```
f  = lambda x : x*np.sin(x)
df = lambda x : np.sin(x) + x*np.cos(x)
D = lambda f,x,h : (f(x+h) - f(x))/h

h = 2**(-np.linspace(0,30,128))
```

```python
plt.title('forward difference')
plt.gca().invert_xaxis();plt.loglog(h,h)
plt.xlabel('h');plt.ylabel('error')
plt.loglog(h,abs((D(f,1.0,h) - df(1.0))/df(1.0)),'.');
```



finite difference approximations

first order approximations of first derivative

Consider the two Taylor series expansions

$$f(x+h) = f(x) + h\, f'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(x) + O\left(h^4\right),$$

and

$$f(x-h) = f(x) - h\, f'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f'''(x) + O\left(h^4\right).$$

- forward difference approximation

$$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h)$$

- backward difference approximation

$$f'(x) = \frac{f(x) - f(x-h)}{h} + O(h)$$

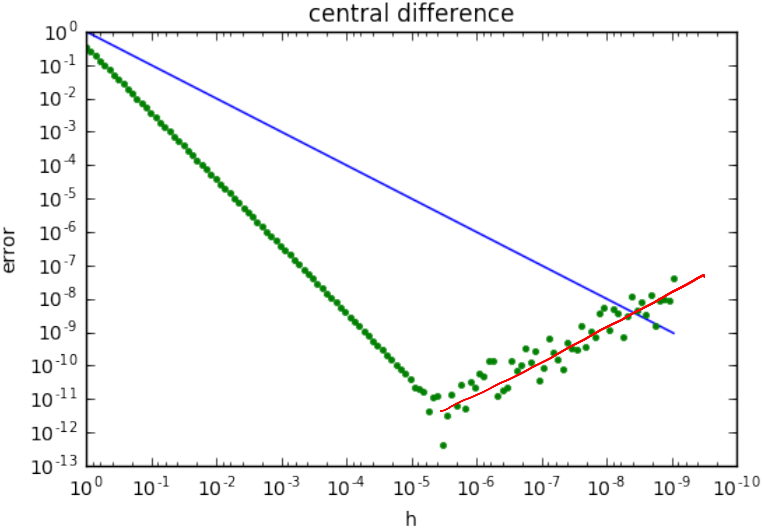
second order approximations of first derivative

- *central difference approximation*

$$f'(x) = \frac{f(x+h) - f(x-h)}{2\,h} - O\Big(h^2\Big)$$

```
Dc = lambda f,x,h : (f(x+h) - f(x-h))/(2*h)
```

```
plt.title("central difference")
plt.gca().invert_xaxis();plt.loglog(h,h);plt.xlabel('h')
plt.ylabel('error');plt.loglog(h,abs((Dc(f,1.0,h) - df(1.0)
```



second derivatives

To find an approximation of the second derivatives further expansion of the Taylor series is required,

$$f(x+h) = f(x) + h\,f'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(x) + \frac{h^4}{24} f''''(x) + O\left(h^5\right),$$

and

$$f(x-h) = f(x) - h\,f'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f'''(x) + \frac{h^4}{24} f''''(x) + O\left(h^5\right)$$

Add the equations to get

$$f(x+h) + f(x-h) = 2\,f(x) + h^2\,f''(x) + \frac{h^4}{12} f''''(x) + O\left(h^5\right)$$

So

$$f''(x) = \frac{f(x+h) - 2\,f(x) + f(x-h)}{h^2} - \frac{h^2\,f''''(x)}{12} + O\left(h^3\right)$$

The Method of Undetermined Coefficients

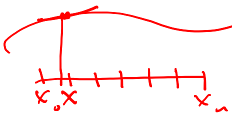
method of undetermined coefficients

- aim: compute approximation $D_h(f,x) \approx f'(x)$ using function values $f(x_k)$ at *grid points* x_k by *finite difference approximation*

$$\boxed{D_h(f,x) = \sum_{k=0}^{n} c_k f(x_k)}$$

- approach: compute coefficients such that formula is exact for polynomials p of degree up to n

$$D_h(p,x) = p'(x)$$



- equidistant grid: consider $x_k = x_0 + kh$
- transformation $z = x_0 + xh$, $g(x) = f(x_0 + xh)$ and

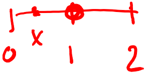
$$g'(x) = hf'(x_0 + xh)$$

- thus determine coefficients c_j for case $\boxed{x_k = k}$ only and use transformation
- special case $x = n/2$: central difference

determination of coefficients c_j for case $x_k = k$ and $n = 2$

- consider monomials $p(x) = 1, x, x^2, \ldots$
- system of equations with Vandermonde matrix

$$\begin{array}{c} x_k^0 \\ x_k^1 \\ x_k^2 \end{array} \underbrace{\begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 2 \\ 0 & 1 & 4 \end{bmatrix}}_{V} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix} = \underbrace{\begin{bmatrix} 0 \\ 1 \\ 2x \end{bmatrix}}_{b}$$



- Gaussian elimination

$$\begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 2 \\ 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 2x - 1 \end{bmatrix} \qquad c_1 = 1 - 2c_2$$

- solution

$$c_2 = x - 1/2, \; c_1 = 2(1 - x), \; c_0 = x - 3/2$$

computing coefficients for central differences

- solve linear system of equations $\boxed{Vc = b}$ where V is Vandermonde matrix with elements k^j
- central differences: $x = n/2$
- Vandermonde matrix using numpy's vander function
- rhs b with components $b_k = k(n/2)^{k-1}$ for $k = 0, 1, \ldots, n$

```
n = 3
V = np.vander(np.arange(n+1),increasing=True).T
b = np.arange(n+1)*(n/2)**(np.arange(n+1)-1)
ck = np.linalg.solve(V,b)
print(ck)
```

```
[ 0.04166667 -1.125       1.125      -0.04166667]
```

example $f'(1)$ for $f(x) = x\sin(x)$ using central difference

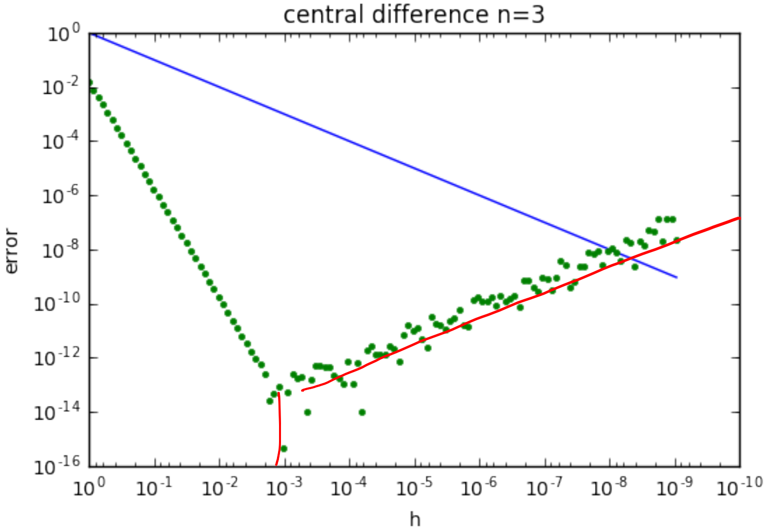
- (transformed) grid points for central difference

$$x_k = 1 + (k - n/2)h$$

- transform coefficients $c_k \to c_k/h$

```
def Dn(f, x, h, ck=ck):
    n = ck.shape[0] - 1
    ydot = 0
    for k in range(n+1):
        ydot += ck[k]/h*f(x+(k-n/2)*h)
    return ydot
```

```python
plt.title("central difference n={}".format(n))
plt.gca().invert_xaxis();plt.loglog(h,h)
plt.xlabel('h');plt.ylabel('error')
plt.loglog(h,abs((Dn(f,1.0,h) - df(1.0))/df(1.0)),'.');
```



Richardson Extrapolation

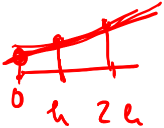
extrapolating central difference

- central difference $\boxed{\phi(h) = (f(x+h) - f(x-h))/(2h)}$
  - $\phi(h)$ is even function, Taylor series contains only terms with h^{2j}
  - if f continuously differentiable, then $\phi(h)$ can be continuously continued so that $\phi(0) = f'(x)$
- interpolating polynomial of $\phi(kh)$ for $k = 1, 2$ as function of k^2 (Lagrange formula!)

$x_1 - x$ $\quad$ $x - x_0$

$$p(k) = \frac{(4-k^2)\phi(h) + (k^2-1)\phi(2h)}{4-1}$$

$x_1 - x_0$



- *extrapolation*: evaluate this polynomial for $k = 0$

$$\boxed{p(0) = \frac{4\phi(h) - \phi(2h)}{3}}$$

extrapolation and elimination

$\varphi(h)$

- Taylor expantions of $f(x \pm h)$ give

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{f'''(x)h^2}{6} + O(h^4)$$

- evaluate this for both h and $2h$

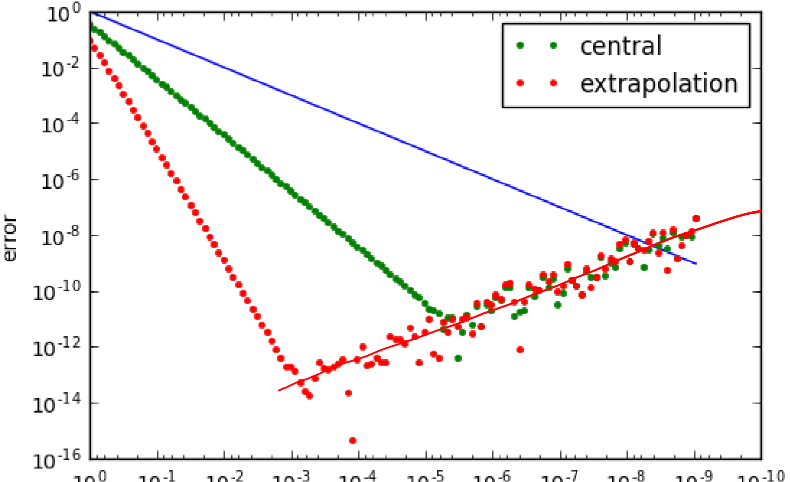
$$f'(x) = \phi(h) + a_2 h^2 + a_4 h^4 + O(h^6)$$
$$f'(x) = \phi(2h) + 4a_2 h^2 + 16a_4 h^4 + O(h^6)$$

- unknowns: $f'(x), a_2, a_4, \ldots$
- idea: eliminate a_2

$$f'(x) = \frac{1}{3}[4\phi(h) - \phi(2h) - 12a_4 h^4] + O(h^6)$$

error of extrapolation

```
R  = lambda f,x,h: (4*Dc(f,x,h) - Dc(f,x,2*h))/3
plt.gca().invert_xaxis();plt.loglog(h,h);plt.xlabel('h');pl
plt.loglog(h,abs((Dc(f,1.0,h) - df(1.0))/df(1.0)),'.',label
plt.loglog(h,abs((R(f,1.0,h) - df(1.0))/df(1.0)),'.',label=
```



Richardson's idea

- sequentially eliminate $a_2, a_4, a_6 \ldots$ by including values $\phi(4k), \phi(8k), \ldots$
- after eliminating a_2 we get

$$f'(x) = \frac{1}{3}[4\phi(h) - \phi(2h) - 12a_4h^4] + O(h^6)$$

- introduce matrix R with $R(n,0) = \phi(2^n h)$ for $n = 0, 1, 2, \ldots$
- furthermore $R(n,1) = (4R(n,0) - R(n+1,0))/3$ so that

$$f'(x) = R(0,1) - 4a_4h^4 + O(h^6)$$

and

2^4

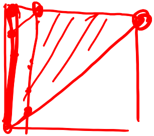
$$f'(x) = R(1,1) - 4^2 * 4a_4h^4 + O(h^6)$$

- now elimnate a_4 to get

$$f'(x) = (4^2R(0,1) - R(1,1))/15 + O(h^6)$$

- thus set $R(n,2) = (4^2R(0,1) - R(1,1))/15$

the general scheme



- start with

$$R(n,0) = \phi(2^n h)$$

$\varphi(h)$ $\varphi(2h)$

- then set

$$R(n,1) = \frac{4R(n,0) - R(n+1,0)}{3}$$

- and repeat to get

$$R(n,k) = \frac{4^k R(n,k-1) - R(n+1,k-1)}{4^k - 1}$$

  until desired accuracy achieved

- show that this eliminates $a_2, a_4, a_6, \ldots$ using Taylor expansion
- this can also be applied to other functions $\phi(h)$

the tableau

- all the $R(i,j)$ required for $R(0,k)$:

$$
\begin{array}{cccccc}
R(0,0) & R(0,1) & R(0,2) & \cdots & \cdots & R(0,k) \\
R(1,0) & R(1,1) & R(1,2) & \cdots & R(1,k-1) & \\
\vdots & \vdots & \vdots & \ddots & & \\
R(k-2,0) & R(k-2,1) & R(k-2,2) & & & \\
R(k-1,0) & R(k-1,1) & & & & \\
R(k,0) & & & & &
\end{array}
$$

- follows from

$$R(n,k) = \frac{4^k R(n,k-1) - R(n+1,k-1)}{4^k - 1}$$

- use $R(n,k)$ for error estimate

$$e_k = R(0,k) - \phi(0) \approx R(0,k) - R(0,k+1)$$

example

```
mr = 5; h = 0.1
R = np.zeros((mr,mr))
for n in range(mr):
    R[n,0] = Dc(f,1.0,2**n*h)
for k in range(1,mr):
    for n in range(mr-k):
        R[n,k] = (4**k*R[n,k-1] - R[n+1,k-1])/(4**k-1)
print(R)
print("exact value: {}".format(df(1.0)))
```

```
[[ 1.37666939  1.38175749  1.38177321  1.38177329  1.381773
 [ 1.36140508  1.38152171  1.38176814  1.38177306  0.
 [ 1.30105517  1.37782526  1.38145793  0.          0.
 [ 1.07074492  1.32333509  0.          0.          0.
 [ 0.3129744   0.          0.          0.          0.
exact value: 1.3817732906760363
```

errors

```
for n in range(mr):
    for k in range(mr-n):
        print("{:1.2e}".format(R[n,k]-df(1.0)),end='   ')
    print("\n")
```

```
-5.10e-03   -1.58e-05   -8.14e-08   -9.07e-10   -2.51e-11

-2.04e-02   -2.52e-04   -5.15e-06   -2.26e-07

-8.07e-02   -3.95e-03   -3.15e-04

-3.11e-01   -5.84e-02

-1.07e+00
```

error approximation for first row in R

```
# error approximation for first row
print("error approx",end='   ')
for k in range(mr-1):
    print("{:1.2e}".format(R[0,k]-R[0,k+1]),end='  ')
print("\n error exact",end='   ')
for k in range(mr-1):
    print("{:1.2e}".format(R[0,k]-df(1.0)),end='  ')
```

```
error approx   -5.09e-03  -1.57e-05  -8.05e-08  -8.82e-10
 error exact   -5.10e-03  -1.58e-05  -8.14e-08  -9.07e-10
```