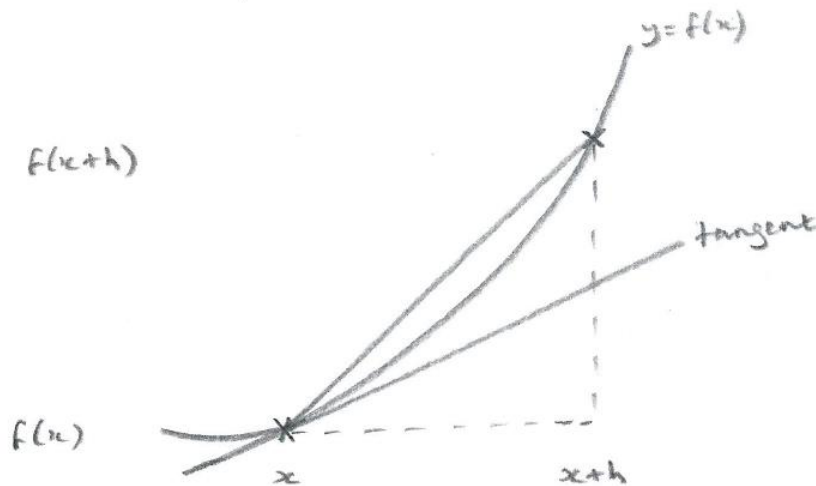


Numerical Differentiation (8 pages; 31/3/20)

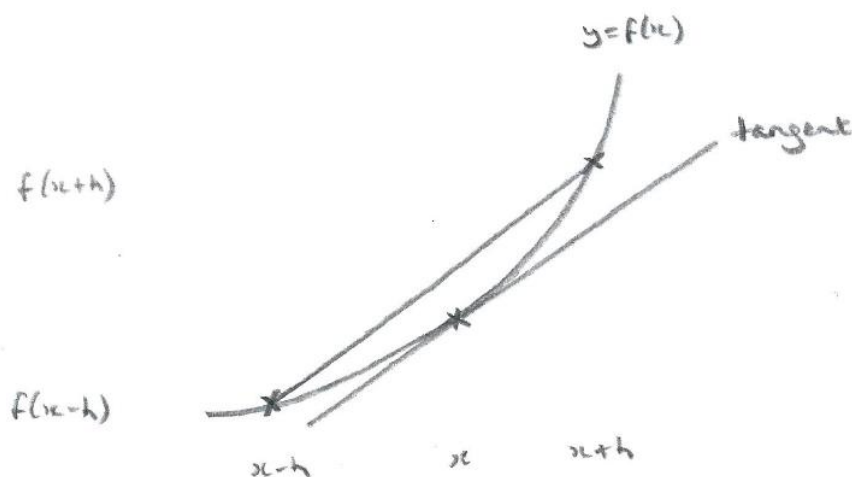
(1) Forward difference approximation to the derivative:

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \quad (\text{for small } h)$$



(2) Central difference approximation to the derivative:

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



(3) Example: $f(x) = \sin x$

To find $f'(1)$ using the forward difference and central difference methods:

	A	B	C
1		$\frac{\sin(1+h) - \sin(1)}{h}$	$\frac{\sin(1+h) - \sin(1-h)}{2h}$
2	h	h	$2h$
3			
4	0.1	0.497363753	0.539402252
5	0.01	0.536085981	0.540293301
6	0.001	0.53988148	0.540302216
7	0.0001	0.540260231	0.540302305
8	0.00001	0.540298099	0.540302306
9	0.000001	0.540301885	0.540302306
10	0.0000001	0.540302264	0.540302306
11	0.00000001	0.540302303	0.540302308

[Actual value: $f'(1) = \cos(1) = 0.540302306$]

(4) Exercise: Find an estimate for $f''(0)$ for $f(x) = \sin x$, using $h = 0.01$, by (i) the Forward difference method, and (ii) the Central difference method.

Solution

$$(i) f''(0) \approx \frac{f'(0.01) - f'(0)}{0.01}$$

$$\text{with } f'(0) \approx \frac{f(0.01) - f(0)}{0.01} = \frac{0.00999983 - 0}{0.01} = 0.999983$$

$$\text{and } f'(0.01) \approx \frac{f(0.02) - f(0.01)}{0.01} = \frac{0.0199987 - 0.00999983}{0.01} = 0.999887,$$

$$\text{so that } f''(0) \approx \frac{0.999887 - 0.999983}{0.01} = -0.0096$$

[The actual value of $f''(0)$ is $-\sin(0) = 0$]

$$(ii) f''(0) \approx \frac{f'(0.01) - f'(-0.01)}{0.02},$$

$$\text{with } f'(-0.01) \approx \frac{f(0) - f(-0.02)}{0.02} = \frac{0 - (-0.0199987)}{0.02} = 0.999935$$

$$\text{and } f'(0.01) \approx \frac{f(0.02) - f(0)}{0.02} = \frac{0.0199987 - 0}{0.02} = 0.999935,$$

$$\text{so that } f''(0) \approx \frac{0.999935 - 0.999935}{0.02} = 0$$

(5) The error for the forward difference can be shown to be approximately proportional to h ; ie it is a "1st order" method. The error for the central difference method can be shown to be approximately proportional to h^2 ; ie it is a "2nd order" method (see Appendix). For this reason, the Central difference method is usually an improvement on the Forward difference method.

(6) A sequence is said to have 1st order convergence if

$$e_{r+1} \approx ke_r \text{ (where } |k| < 1), \text{ where } e_r = x_r - \alpha$$

2nd order convergence is when $e_{r+1} \approx ke_r^2$ (again, with $|k| < 1$)

In the case of 1st order convergence, we can show that

$$\frac{x_{r+1} - x_r}{x_r - x_{r-1}} \text{ (the 'ratio of differences')} \approx k$$

Proof

$$e_r = x_r - \alpha \text{ and } e_{r+1} = x_{r+1} - \alpha$$

$$e_r \approx ke_{r-1} \text{ and } e_{r+1} \approx ke_r$$

$$\text{So } \frac{x_{r+1} - x_r}{x_r - x_{r-1}} = \frac{(\alpha + e_{r+1}) - (\alpha + e_r)}{(\alpha + e_r) - (\alpha + e_{r-1})} = \frac{e_{r+1} - e_r}{e_r - e_{r-1}} = \frac{ke_r - ke_{r-1}}{e_r - e_{r-1}} \approx k$$

$$(7) \text{ Let } fd(h) = \frac{f(x+h)-f(x)}{h}$$

As the forward difference method is a 1st order method,

$$\frac{fd\left(\frac{h}{2^n}\right)-f'(x)}{fd\left(\frac{h}{2^{n-1}}\right)-f'(x)} \approx \frac{\lambda\left(\frac{h}{2^n}\right)}{\lambda\left(\frac{h}{2^{n-1}}\right)} = \frac{1}{2}$$

Thus $e_n \approx \frac{1}{2}e_{n-1}$, where $e_n = x_n - \alpha$, with $x_n = fd\left(\frac{h}{2^n}\right)$

and $\alpha = f'(x)$,

and so the forward difference method has 1st order convergence.

Hence, from the 'ratio of differences' result, $\frac{fd\left(\frac{h}{4}\right)-fd\left(\frac{h}{2}\right)}{fd\left(\frac{h}{2}\right)-fd(h)} \approx \frac{1}{2}$

$$\Rightarrow fd\left(\frac{h}{4}\right) - fd\left(\frac{h}{2}\right) \approx \frac{1}{2}(fd\left(\frac{h}{2}\right) - fd(h)) \quad (1)$$

$$\Rightarrow fd\left(\frac{h}{4}\right) \approx fd\left(\frac{h}{2}\right) + \frac{1}{2}(fd\left(\frac{h}{2}\right) - fd(h)) \quad (1')$$

ie given $fd(h)$ & $fd\left(\frac{h}{2}\right)$, we can estimate $fd\left(\frac{h}{4}\right)$ (which will be a better estimate for $f'(x)$)

$$\text{Similarly, } fd\left(\frac{h}{8}\right) \approx fd\left(\frac{h}{4}\right) + \frac{1}{2}(fd\left(\frac{h}{4}\right) - fd\left(\frac{h}{2}\right)) \quad (1'')$$

So, from (1') & (1),

$$fd\left(\frac{h}{8}\right) \approx \left[fd\left(\frac{h}{2}\right) + \frac{1}{2}\left(fd\left(\frac{h}{2}\right) - fd(h)\right)\right]$$

$$+ \frac{1}{2} \cdot \frac{1}{2}(fd\left(\frac{h}{2}\right) - fd(h)) \quad (2)$$

$$\text{And } fd\left(\frac{h}{16}\right) \approx fd\left(\frac{h}{8}\right) + \frac{1}{2}(fd\left(\frac{h}{8}\right) - fd\left(\frac{h}{4}\right)) \quad (3)$$

so that, from (3) & (2)

$$fd\left(\frac{h}{16}\right) \approx \left[fd\left(\frac{h}{2}\right) + \frac{1}{2}\left(fd\left(\frac{h}{2}\right) - fd(h)\right) + \frac{1}{2^2}\left(fd\left(\frac{h}{2}\right) - fd(h)\right) \right] \\ + \frac{1}{2} \cdot \frac{1}{2}\left(fd\left(\frac{h}{4}\right) - fd\left(\frac{h}{2}\right)\right)$$

$$[\text{as } fd\left(\frac{h}{8}\right) - fd\left(\frac{h}{4}\right) \approx \frac{1}{2}\left(fd\left(\frac{h}{4}\right) - fd\left(\frac{h}{2}\right)\right), \text{ from (1'')}]$$

$$\approx fd\left(\frac{h}{2}\right) + \frac{1}{2}\left(fd\left(\frac{h}{2}\right) - fd(h)\right) + \frac{1}{2^2}\left(fd\left(\frac{h}{2}\right) - fd(h)\right)$$

$$+ \frac{1}{2^3}\left(fd\left(\frac{h}{2}\right) - fd(h)\right), \text{ from (1)}$$

So, by repeating this process,

$$f'(x) \approx fd\left(\frac{h}{2}\right) + \frac{1}{2}\left(fd\left(\frac{h}{2}\right) - fd(h)\right) + \frac{1}{2^2}\left(fd\left(\frac{h}{2}\right) - fd(h)\right)$$

$$+ \frac{1}{2^3}\left(fd\left(\frac{h}{2}\right) - fd(h)\right) + \dots$$

$$\approx fd\left(\frac{h}{2}\right) + \frac{1}{2}\left(fd\left(\frac{h}{2}\right) - fd(h)\right) \frac{1}{1-\frac{1}{2}}$$

$$= fd\left(\frac{h}{2}\right) + \left(fd\left(\frac{h}{2}\right) - fd(h)\right)$$

Naturally we would use the best pair of forward difference estimates available,

$$\text{when } f'(x) \approx fd\left(\frac{h}{2^n}\right) + \left(fd\left(\frac{h}{2^n}\right) - fd\left(\frac{h}{2^{n-1}}\right)\right)$$

$$\text{or } 2fd\left(\frac{h}{2^n}\right) - fd\left(\frac{h}{2^{n-1}}\right)$$

Note: The same result can be obtained more simply as follows:

$$\frac{fd\left(\frac{h}{2^n}\right) - f'(x)}{fd\left(\frac{h}{2^{n-1}}\right) - f'(x)} \approx \frac{1}{2} \Rightarrow 2fd\left(\frac{h}{2^n}\right) - 2f'(x) \approx fd\left(\frac{h}{2^{n-1}}\right) - f'(x)$$

$$\Rightarrow f'(x) \approx 2fd\left(\frac{h}{2^n}\right) - fd\left(\frac{h}{2^{n-1}}\right)$$

$$(8) \text{ Let } cd(h) = \frac{f(x+h) - f(x-h)}{2h}$$

As the central difference method is a 2nd order method,

$$\frac{cd\left(\frac{h}{2^n}\right) - f'(x)}{cd\left(\frac{h}{2^{n-1}}\right) - f'(x)} \approx \frac{\lambda\left(\frac{h}{2^n}\right)^2}{\lambda\left(\frac{h}{2^{n-1}}\right)^2} = \frac{1}{4}$$

and so the central difference method has 1st order convergence,

$$\text{as } e_n \approx \frac{1}{4} e_{n-1}$$

[Note the confusing terminology: 2nd order method, but 1st order convergence.]

In the same way as for the forward difference method, this leads to

$$f'(x) \approx cd\left(\frac{h}{2}\right) + \frac{1}{4}\left(cd\left(\frac{h}{2}\right) - cd(h)\right) + \frac{1}{4^2}\left(cd\left(\frac{h}{2}\right) - cd(h)\right)$$

$$+ \frac{1}{4^3}\left(cd\left(\frac{h}{2}\right) - cd(h)\right) + \dots$$

$$\approx cd\left(\frac{h}{2}\right) + \frac{1}{4}\left(cd\left(\frac{h}{2}\right) - cd(h)\right) \frac{1}{1 - \frac{1}{4}}$$

$$= cd\left(\frac{h}{2}\right) + \frac{1}{3}\left(cd\left(\frac{h}{2}\right) - cd(h)\right)$$

and more generally:

$$f'(x) \approx cd\left(\frac{h}{2^n}\right) + \frac{1}{3}\left(cd\left(\frac{h}{2^n}\right) - cd\left(\frac{h}{2^{n-1}}\right)\right)$$

$$\text{or } \frac{4}{3}cd\left(\frac{h}{2^n}\right) - \frac{1}{3}cd\left(\frac{h}{2^{n-1}}\right)$$

Appendix

(i) Proof that Forward Difference method is a 1st order method

One of the forms of the Taylor expansion of a function is

$$f(x + a) = f(a) + xf'(a) + \frac{x^2 f''(a)}{2!} + \frac{h^3 f'''(a)}{3!} + \dots$$

(using the notation of "Taylor Series")

This can be rewritten as

$$f(h + x_0) = f(x_0) + hf'(x_0) + \frac{h^2 f''(x_0)}{2!} + \frac{h^3 f'''(x_0)}{3!} + \dots$$

and it can be shown that $\frac{h^2 f''(x_0)}{2!} + \frac{h^3 f'''(x_0)}{3!} + \dots = \frac{h^2 f''(\eta)}{2!}$,

where $x_0 < \eta < x_0 + h$,

so that $f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2 f''(\eta)}{2!}$

and hence $\frac{f(x_0+h)-f(x_0)}{h} = f'(x_0) + \frac{hf''(\eta)}{2!}$

Thus the error term $\frac{f(x_0+h)-f(x_0)}{h} - f'(x_0)$ is approximately proportional to h [as $f''(\eta)$ will tend to $f''(x)$]; ie is of order h (or $O(h)$), and so the Forward Difference method is a 1st order method (because the error is of order h^1).

(ii) Proof that Central Difference method is a 2nd order method

It can also be shown that

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2 f''(x_0)}{2!} + \frac{h^3 f'''(\eta_1)}{3!}, \text{ where}$$

$$x_0 < \eta_1 < x_0 + h$$

Also $f(x_0 - h) = f(x_0) + (-h)f'(x_0) + \frac{(-h)^2 f''(x_0)}{2!} + \frac{(-h)^3 f'''(\eta_2)}{3!}$

Then $f(x_0 + h) - f(x_0 - h) = 2hf'(x_0) + \frac{h^3[f'''(\eta_1) + f'''(\eta_2)]}{3!}$

and hence $\frac{f(x_0+h) - f(x_0-h)}{2h} = f'(x_0) + \frac{h^2[f'''(\eta_1) + f'''(\eta_2)]}{12}$

Thus the error term for the Central Difference method is approximately proportional to h^2 (ie is $O(h^2)$), and so it is a 2nd order method.