Lecture 8

Last time we did Richardson Extrapolation

This consists of using two lower order approximations to create a higher order approximation

$$M = N(h) + K_1 h + K_2 h^2 + \cdots + K_n h^n + \cdots$$

h sufficiently small

$$M = N(h/2) + K_1 h/2 + K_2 h^2/4 + \cdots$$

One can eliminate $K_1 h$ to get $O(h^2)$ formula

Iterating this procedure $O(h^n)$ formula for M can be found

We then studied Romberg integration

This is Richardson extrapolation applied to composite trapezoidal rule

$$I = \int_a^b f(x)\,dx$$

$$N = \frac{b-a}{h}$$

$$T_N = \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{N-1} f(x_i) + f(x_N) \right]$$

$$I = T_N + K_2 h^2 + K_4 h^4 + K_6 h^6 + \cdots$$

$$I = T_{2N} + K_2 \frac{h^2}{4} + K_4 \frac{h^4}{16} + \cdots$$

One eliminates $K_2 h^2$ to get $O(h^4)$ approximation to I.

Iterating $O(h^{2n})$ formulas to I can be found.

Numerical Differentiation

$f: [a,b] \to \mathbb{R}$ is given

We need to compute $f'(x)$.

This is usually done when $f(x)$ is not known analytically

Only a table of function values is known

Note the methods of Numerical differentiation have applications in the study of Ordinary differential equations

$$f'(a) = \lim_{h \to 0} \frac{f(a+h) - f(a)}{h}$$

Thus $\frac{f(a+h)-f(a)}{h}$ is our first initial approximation to the derivative.

(Note h can be $-ve$)

Example

$f(x) = \sin x$

x	$f(x)$	Approximate $f'(x)$	Exact
0.2	0.1987	0.9680	0.9801
0.3	0.2955	0.9390	0.9553
0.4	0.3894	0.9000	0.9211
0.5	0.4794	0.9000	0.8776

Remark ① We use $h = 0.1$ to compute $f'(0.2)$, $f'(0.3)$, $f'(0.4)$

We used $h = -0.1$ to compute $f'(0.5)$

Remark :- Our approximation to $f'(a)$ is correct upto only one significant digit

- Higher accuracy may be obtained by Richardson Extrapolation
- We need error estimates

Basic idea of techniques for numerical differentiation

$$f(x) \approx P_k(x)$$

$P_k(x)$ interpolates $f(x)$ at $x_0, x_1, \ldots, x_k$.

Then $f'(x) \approx P_k'(x)$

Let $f : [a, b] \longrightarrow \mathbb{R}$ be continuously differentiable. Let $x_0, x_1, \ldots, x_k$ be distinct points in $[a, b]$

$$f(x) = P_k(x) + f[x_0, x_1, \ldots, x_k, x]\,\psi_k(x)$$

$$\psi_k(x) = \prod_{i=0}^{k} (x - x_i)$$

$$f'(x) = P_k'(x) + \left(\frac{d}{dx} f[x_0, x_1, \ldots, x_k, x]\right)\psi_k(x) + f[x_0, x_1, \ldots, x_k, x]\,\psi_k'(x)$$

$$\frac{d}{dx} f[x_0, x_1, \ldots, x_k, x]$$

$$= \lim_{y \to x} \frac{f[x_0, x_1, \ldots, x_k, y] - f[x_0, x_1, \ldots x_k, x]}{y - x}$$

$$= f[x_0, x_1, \ldots, x_k, x, x] \quad [\text{Exercise}]$$

Thus $f'(x) = P_k'(x) + f[x_0, \ldots x_k, x, x]\,\psi_k(x) + f[x_0, \ldots, x_k]\,\psi_k'(x)$

We approximate $f'(a)$ by $P'(a)$

$$\text{Error} = f[x_0, \ldots x_k, a, a]\,\psi_k(a) + f[x_0, \ldots, x_k, a]\,\psi_k'(a)$$

$$E(f)_a = \frac{f^{(k+2)}(\xi)}{(k+2)!}\,\psi_k(a) + \frac{f^{(k+1)}(\eta)}{(k+1)!}\,\psi_k'(a)$$

for some $\xi, \eta \in (c, d)$

This expression tell us very little about the true error, since in practise we usually do not know $f^{(k+1)}$ and $f^{(k+2)}$ involved in $E(f)$ and we will almost never know ξ, n

So we try to find situations where the error term can be simplified

Case 1 a is one of the interpolating points

$a = x_i$

Since $\psi_k(x)$ contains factor $(x - x_i)$

we get $\psi_k(a) = 0$

So first term in error drops out.

Moreover $\psi_k'(a) = q(a)$

where $q(x) = \dfrac{\psi_k(x)}{x - x_i}$

$$= \prod_{\substack{j=0 \\ j \neq i}}^{k} (x - x_i)$$

Thus $E(f) = \dfrac{f^{(k+1)}(\eta)}{(k+1)!} \prod_{\substack{j=0 \\ j \neq k}}^{k} (x_i - x_j)$

Case(2) $\psi_k'(a) = 0$. (we choose a with this property)

$k \to$ odd

then we can achieve this by placing x_i's symmetrically around a, so that

$x_{k-j} - a = a - x_j \qquad j = 0, 1, \ldots, \frac{k-1}{2}$

Then

$$(x-x_j)(x-x_{k-j}) = (x-a)^2 - (a-x_j)^2$$

$$j = 0, 1, \ldots, \frac{k-1}{2}$$

$$\psi_k(x) = \prod_{j=0}^{\frac{k-1}{2}} \left[(x-a)^2 - (a-x_j)^2 \right]$$

$$\frac{d}{dx}\left[(x-a)^2 - (a-x_j)^2 \right] \Big|_{x=a} = 0$$

So $\psi_k'(a) = 0$

Thus in this case

$$E(f) = \frac{1}{(k+2)!} f^{(k+2)}(\xi) \prod_{j=0}^{\frac{k-1}{2}} \left[-(a-x_j)^2 \right]$$

Specific Examples

$k=1$

$$P_k(x) = f(x_0) + f[x_0, x_1](x - x_0)$$

$$P_k'(x) = f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

Case(1) $a = x_0$ and $h = x_1 - x_0$

we get $f'(a) \approx f[a, a+h] = \frac{f(a+h) - f(a)}{h}$

$$E(f) = -\frac{1}{2} h f''(\eta)$$

Case(2) $a = \frac{x_0 + x_1}{2}$.

x_0 and x_1 are symmetric w.r.t a

$x_0 = a - h$, $x_1 = a + h$, $h = \frac{1}{2}(x_1 - x_0)$

we get central difference formula

$$f'(a) \approx f[a-h, a+h] = \frac{f(a+h) - f(a-h)}{2h}$$

$$E(f) = -\frac{h^2}{6} f'''(\xi)$$

This is $O(h^2)$ approximation.

Next we consider using three interpolating points

$$P_2(x) = f(x_0) + f[x_0, x_1](x - x_1) + f[x_0, x_1, x_2](x - x_0)(x - x_1)$$

$$P_2'(x) = f[x_0, x_1] + f[x_0, x_1, x_2](2x - x_0 - x_1)$$

$$x_0 = a, \quad x_1 = a+h, \quad x_2 = a+2h$$

$$f'(a) \approx \frac{-3f(a) + 4f(a+h) - f(a+2h)}{2h} \quad (2)$$

$$E(f) = \frac{h^2}{3} f'''(\xi) \quad \text{for some} \quad (*)$$

ξ between a and $a+2h$

Remark :- Central diff formula

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

has error $-\frac{h^2}{6} f'''(\eta)$

is usually less than $(*)$

However (2) is used when a is beginning or end of a table

Example

$f(x) = \sin x$

x	f(x)	Formula 1	Form ②	Form 3	Exact
0.2	1.987 E-1	9.685 E-1	-	9.833 E-1	9.801 E-1
0.3	2.955 E-1	9.390 E-1	9.537 E-1	9.584 E-1	9.553 E-1
0.4	3.894 E-1	9.001 E-1	9.195 E-1	9.240 E-1	9.211 E-1
0.5	4.794 E-1	8.522 E-1	8.761 E-1	8.804 E-1	8.776 E-1
0.6	5.646 E-1	7.958 E-1	8.240 E-1	8.279 E-1	8.253 E-1
0.7	6.442 E-1	7.314 E-1	7.636 E-1	7.675 E-1	7.648 E-1
0.8	7.174 E-1	7.314 E-1	—	6.992 E-1	6.967 E-1

form (1) (*) $f'(a) \approx \dfrac{f(a+h) - f(a)}{h}$

form (2) $f'(a) \approx \dfrac{f(a+h) - f(a-h)}{2h}$

form (3) (*) $f'(a) \approx \dfrac{-3f(a) + 4f(a+h) - f(a+2h)}{2h}$

(*) at ends of table use take $h = -0.1$

Formula ② is best whenever it is applicable. Formula ③ is better then formula ① at endpoints.

Central difference formula for second derivative $f \in C^4$

$$f(x_0+h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_1)h^4$$

$$f(x_0-h) = f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 - \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_2)h^4$$

where $x_0 - h < \xi_2 < x_0 < \xi_1 < x_0 + h$

$$f(x_0+h) + f(x_0-h) = 2f(x_0) + f''(x_0)h^2 + \frac{1}{24}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_2)\right]h^4$$

Note $f^{(4)}$ is continuous by assumption

$\frac{1}{2}\left[f^4(\xi_1) + f^4(\xi_2)\right]$ is between $f^{(4)}(\xi_1)$ and $f^{(4)}(\xi_2)$

so $\frac{1}{2}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_2)\right] = f^{(4)}(\xi)$

for some $\xi \in (x_0-h, x_0+h)$

Thus

$$f''(x_0) = \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2} - \frac{h^2}{12} f^{iv}(\xi)$$

Errors associated to computation of derivative

$$f'(a) \approx \underbrace{\frac{f(a+h) - f(a-h)}{2h}}_{\text{approximation}} + \underbrace{\left(-\frac{h^2}{6}\right) f'''(\xi)}_{\text{Error (discretization error)}}$$

Theoretically it might seem that as h becomes small then $f'(a)$ can be computed with high degree of accuracy

However as h is small $\frac{f(a+h) - f(a-h)}{2h}$

creates loss of sig digits and there is loss of accuracy because of this

Example $f(x) = e^x$

$a = 0$

h	e^h	e^{-h}	$\frac{e^h - e^{-h}}{2h}$
~~2.1~~	~~2.718~~		
0.1	1.10517	9.04837 E-1	1.00167
0.05	1.05127	9.51229 E-1	1.00041
0.01	1.01005	9.90050 E-1	1.00000
0.005	1.00501	9.95012 E-1	9.99800 E-1
0.001	1.00100	9.99 E-1	1.00000
0.0005	1.00050	9.99500 E-1	1.0000
0.0001	1.00010	9.99900 E-1	1.0000
0.00001	1.00001	9.99990 E-1	1.00000
0.000001	1.00000	9.99999 E-1	0.5
1E-7	1.00000	1.00000	0

error jumps

Analysis of this phenomenon.

$$f'(a) = \frac{f(a+h) - f(a-h)}{2h} - \frac{h^2 f^{(3)}(\xi)}{6}$$

In calculation $f(a+h) + E_+$ will be computed
$f(a+h) - E_-$ (due to Round off)

$$f'_{comp} = \frac{f(a+h) + E_+ - f(a-h) + E_-}{2h}$$

$$= \frac{f(a+h) - f(a-h)}{2h} + \frac{E_+ + E_-}{2h}$$

So $$\underbrace{f'(a)}_{\text{Exact}} = \underbrace{f'_{comp}}_{\text{Approx}} - \frac{E_+ + E_-}{2h} - \frac{h^2 f^{(3)}(\xi)}{6}$$

$\frac{E_+ + E_-}{2h}$: increases as $h \to 0$

$\frac{h^2 f^{(3)}(\xi)}{6}$: decreases as $h \to 0$

Thus Numerical differentiation is an unstable process.

How to improve accuracy of computing derivatives

- Use Richardson Extrapolation.

$$f'(a) \doteq \frac{f(a+h)-f(a)}{h} + K_1 h + K_2 h^2 + \cdots + K_n h^n + \cdots$$

h suff small
K_i constant

$$f'(a) = \frac{f(a+h)-f(a-h)}{2h} + K_2 h^2 + K_4 h^4 + \cdots + K_{2n} h^{2n} + \cdots$$

h suff small
K_i constant

Example $f(x) = \sin x + \cos x$

$a = 0.3$

$N_1(h) = \dfrac{f(a+h)-f(a-h)}{2h}$

h	$N_1(h)$	$N_2(h)$	$N_3(h)$
0.1	6.5872E-1		
0.05	6.5954E-1		
0.025	6.5975E-1		
0.0125	6.5980E-1		

Example $f(x) = \sin x + \cos x$

$a = 0.3$

$$N_1(h) = \frac{f(a+h) - f(a-h)}{2h}$$

computation with 6 sig digits

h	$N_1(h)$	$N_2(h)$	$N_3(h)$	$N_4(h)$
0.1	6.58717 E-1			
0.05	6.59541 E-1	6.59816 E-1		
0.025	6.59748 E-1	6.59817 E-1	6.59817 E-1	
0.0125	6.59799 E-1	6.59816 E-1	6.59816 E-1	6.59816 E-1

Exact upto 6 sig digits $f'(0.3) = \cos 0.3 - \sin 0.3$

$= 6.59816 \text{ E-1}$

Thus our answer is correct upto 6 sig digits.

Note $N_1(0.0125)$ is correct upto only 4 sig digits.

Application of formulas for numerical differentiation to solve ↓ Boundary-value problems in O.D.E. linear

$$y''(x) + f(x)y'(x) + g(x)y = q(x)$$

$$y(a) = \alpha \qquad x \in [a, b].$$
$$y(b) = \beta$$

$$h = \frac{b-a}{N} \qquad x_0 = a$$
$$x_i = x_0 + ih$$
$$i = 1, \dots, N$$

We use central difference approximation

$$y(x_i) = y_i$$

$i = 1, 2, \dots, N-1$

$$\frac{y_{i-1} - 2y_i + y_{i+1}}{h^2} + \frac{f(x_i)(y_{i+1} - y_{i-1})}{2h}$$

$$+ g(x_i)y_i = q(x_i)$$

$$i = 1, 2, \dots, N-1$$

Multiplying by h^2 and setting $f(x_i) = f_i$
$g(x_i) = g_i$
$q(x_i) = q_i$

and grouping terms we get

$$\left(1-\frac{h}{2}f_i\right)y_{i-1} + (-2+h^2 g_i)\,y_i + \left(1+\frac{h}{2}f_i\right)y_{i+1} = h^2 g_i$$

$$i = 1, 2, \ldots, N-1$$

as y_0 and y_N are known

this is a $(n-1)\times(n-1)$ system.

$$A\begin{bmatrix} y_1 \\ \vdots \\ y_{N-1} \end{bmatrix} = b$$

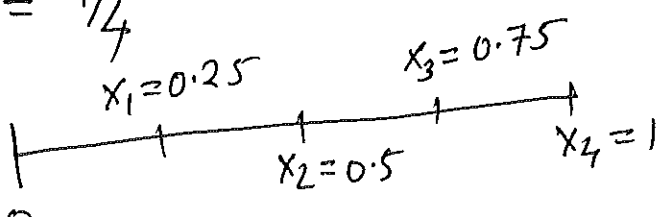
A is a tridigonal matrix
i.e entries in diagonal and
above diagonal and below
diagonal entries
only.

Example

$$\frac{d^2y}{dx^2} + y = 0$$

$$y(0) = 0 \qquad y(1) = 1$$

$h = 1/4$



Approximate y_1, y_2, y_3 and compare with exact $y(x) = \dfrac{\sin x}{\sin 1}$.

$$\frac{y_0 - 2y_1 + y_2}{h^2} + y_1 = 0 \qquad i=1$$

$$\frac{y_1 - 2y_2 + y_3}{h^2} + y_2 = 0 \qquad i=2$$

$$\frac{y_2 - 2y_3 + y_4}{h^2} + y_3 = 0 \qquad i=3$$

$y_0 = 0 \qquad y_4 = 1$

multiply ①, ② ③ by h^2 and rearrange

$$(-2+h^2)y_1 + y_2 + 0y_3 = 0$$

$$y_1 + (-2+h^2)y_2 + y_3 = 0$$

$$0y_1 + y_2 + (-2+h^2)y_3 = -1$$

$$-2 + h^2 = -1.9375$$

Exact $y = \frac{\sin x}{\sin 1}$

$y_1 = 2.94014\ E{-1}$

$y_2 = 5.69747\ E{-1}$

$y_3 = 8.10056\ E{-1}$

In six sig digits

Approx

$y_1 = 2.94274\ E{-1}$

$y_2 = 5.70156\ E{-1}$

$y_3 = 8.10403\ E{-1}$

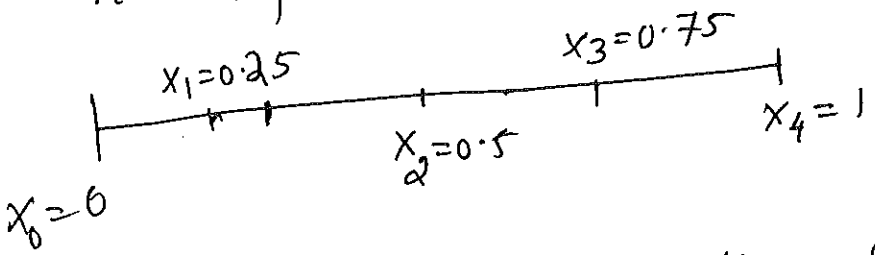
Our answers are correct upto 3 sig digits.

Exercise Solve

$$\frac{d^2y}{dx^2} + \frac{dy}{dx} = 0$$

$$y(0) = 0 \qquad y(1) = 1$$

$h = 1/4$



Approximate y_1, y_2, y_3 and compare with exact

$$y(x) = \frac{1}{1-e^{-1}}(1 - e^{-x})$$

$$\frac{y_0 - 2y_1 + y_2}{h^2} + \frac{y_2 - y_0}{2h} = 0 \qquad i=1$$

$$\frac{y_1 - 2y_2 + y_3}{h^2} + \frac{y_3 - y_1}{2h} = 0 \qquad i=2$$

$$\frac{y_2 - 2y_3 + y_4}{h^2} + \frac{y_4 - y_2}{2h} = 0 \qquad i=3$$

①, ②, ③ $\times h^2$ and rearrange

Also use $y_0 = 0$ $\quad y_1 = 1$

$$-2y_1 + \frac{h}{2} y_2 + 0\, y_3 = 0$$

$$\left(1 - \frac{h}{2}\right) y_1 - 2y_2 + \left(1 + \frac{h}{2}\right) y_3 = 0$$

$$0\, y_1 + \left(1 - \frac{h}{2}\right) y_2 - 2y_3 = -1 - \frac{h}{2}$$

$h = 0.25$ $\quad h/2 = 0.125$

exact $y = \frac{1}{1-e^{-1}} (1 - e^{-x})$

Computed	exact
$y_1 = 2.72177\ E{-2}$	$y_1 = 3.49932\ E{-1}$
$y_2 = 4.35484\ E{-1}$	$y_2 = 6.22459\ E{-1}$
$y_3 = 7.53024\ E{-1}$	$y_3 = 8.34704\ E{-1}$

Not a single digit accuracy.
so have to take h smaller

~~How~~

Remark :- If we take h too big we have lot of discretization error.

If we take h too small then we have lot of round-off error.

A partial solution is to use Richardson extrapolation.

It can be shown that

$$y(x_i) = y^{approx}(x_i) + K_2 h^2 + K_4 h^4 + K_6 h^6 + \cdots$$

One can eliminate K_2 and get $O(h^4)$ approximations.