Numerical Analysis : [MA214]
Lecture 8

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Recall

Last time we did Richardson Extrapolation
This consists of using two lower approximations to create a higher order approximation

$$M = N(h) + k_1 h + k_2 h^2 + k_3 h^3 + \cdots + k_n h^n + \cdots$$

(h sufficiently small)

$$M = N(h/2) + k_1 \frac{h}{2} + k_2 \frac{h^2}{4} + \cdots$$

One can elimate $k_1 h$ 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.

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

$$N = \frac{b-a}{h} \ , \ x_i = a + ih \ , \ i = 0, 1, \cdots , N$$

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

$$I = T_N + k_2 h^2 + k_4 h^4 + k_6 h^6 + \cdots$$

$$I = T_{2N} + k_2 \frac{h^2}{4} + k_4 \frac{h^4}{16} + \cdots$$

One eliminates $k_2 h^2$ to get $O(h^4)$ approximation to I.

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

Numerical Differentiation

$f : [a, b] \longrightarrow \mathbb{R}$ 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 that the method 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 have negative value

Example:- $f(x) = sinx$

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

Remarks:-

1. We use $h = 0.1$ to compute $f'(0.2)$, $f'(0.3)$, $f'(0.4)$ and we use $h = -0.1$ to compute $f'(0.5)$.
2. Our approximation to $f'(a)$ is correct upto only one significant digit.
3. Higher accuracy may be obtained by Richardson extrapolation.
4. We need error estimates

Basic idea of techniques for numerical differentiation

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

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

Then $f'(x) \approx P'_k(x)$

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

$$\begin{aligned}
f(x) &= P_k(x) + f[x_0, x_1, \cdots, x_k, x]\Psi_k(x) \\
&\text{where } \Psi_k(x) = \prod_{i=0}^{k}(x - x_i) \\
f'(x) &= P'_k(x) + \left(\frac{d}{dx} f[x_0, x_1, \cdots, x_k, x]\right)\Psi_k(x) \\
&+ f[x_0, x_1, \cdots, x_k, x]\Psi'_k(x)
\end{aligned}$$

$$
\begin{aligned}
\frac{d}{dx} f[x_0, x_1, \cdots, x_k, x] &= \lim_{y \to x} \frac{f[x_0, x_1, \cdots, x_k, y] - f[x_0, x_1, \cdots, x_k, x]}{y - x} \\
&= f[x_0, x_1, \cdots, x_k, x, x]
\end{aligned}
$$

Thus

$$
f'(x) = P'_k(x) + f[x_0, x_1, \cdots, x_k, x, x]\Psi_k(x) + f[x_0, x_1, \cdots, x_k, x]\Psi'_k(x)
$$

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

$$
\begin{aligned}
Error &= f[x_0, x_1, \cdots, x_k, a, a]\Psi_k(a) + f[x_0, x_1, \cdots, x_k, a]\Psi'_k(a) \\
E(f)_a &= \frac{f^{(k+2)}(\xi)}{(k+2)!}\Psi_k(a) + \frac{f^{(k+1)}(\eta)}{(k+1)!}\Psi'_k(a)
\end{aligned}
$$

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

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

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

Case 1 :- a is one of the interpolating points

$$a = x_i$$

Since $\Psi_k(a)$ 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

$$q(x) = \frac{\Psi_k(x)}{x - x_i} = \prod_{j=0, j \neq i}^{k} (x - x_j)$$

Thus

$$E(f) = \frac{f^{(k+1)}(\eta)}{(k+1)!} \prod_{j=0, j\neq i}^{k} (x_i - x_j)$$

Case 2 :- $\Psi_k'(a) = 0$, (we choose a with this property)

$k \to odd$, then we can achieve this by playing x_i's symmetrically around a, so that

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

Then

$$(x - x_j)(x - x_{k-j}) = (x-a)^2 - (a - x_j)^2 \ , \ j = 0, 1, \cdots , \frac{k-1}{2}$$

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

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

So $\Psi_k'(a)=0$ Thus in this case

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

$k = 1$

$$\begin{aligned} P_k(x) &= f(x_0) + f[x_0, x_1](x - x_0) \\ P_k'(x) &= f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0} \end{aligned}$$

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

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

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

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

Next we consider using three interpolating points.

$$\begin{aligned} P_2(x) &= f(x_0) + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) \\ P_2'(x) &= f[x_0, x_1] + f[x_0, x_1, x_2](2x - x_0 - x_1) \end{aligned}$$

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

$$f'(a) \approx \frac{-3f(a) + 4f(a+h) - f(a+2h)}{2h} \tag{1}$$

$$E(f) = \frac{h^2}{3} f^{(3)}(\xi) \tag{2}$$

for some ξ between a and $a + 2h$

Remark:- Central Diff. formula

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

has error $-\frac{h^2}{6} f^{(3)}(\eta)$ is usually less then equation (2).

However equation (1) is used when a is beginning or ending a table.

Example

$$f(x) = sinx$$

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

$$
\begin{aligned}
&form-1 \quad f'(a) \approx \quad \frac{f(a+h)-f(a)}{h}\\
&form-2 \quad f'(a) \approx \quad \frac{f(a+h)-f(a-h)}{2h}\\
&form-3 \quad f'(a) \approx \quad \frac{-3f(a)+4f(a+h)-f(a+2h)}{2h}
\end{aligned}
$$

at ends of table we take $h=-0.1$

Formula-2 is best whenever it is applicable. Formula-3 is better then formula-1 at end points.

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

$$
\begin{aligned}
f(x_0+h) &= f(x_0) + f'(x_0)h + \frac{1}{2!}f''(x_0)h^2 \\
&+ \frac{1}{3!}f^{(3)}(x_0)h^3 + \frac{1}{4!}f^{(4)}(\xi_1)h^4 \\
f(x_0-h) &= f(x_0) - f'(x_0)h + \frac{1}{2!}f''(x_0)h^2 \\
&- \frac{1}{3!}f^{(3)}(x_0)h^3 + \frac{1}{4!}f^{(4)}(\xi_2)h^4 \\
\text{where} \quad & x_0 - h < \xi_2 < x_0 < \xi_1 < x_0 + h \\
f(x_0+h) + f(x_0-h) &= 2f(x_0) + f''(x_0)h^2 + \frac{1}{4!}[f^{(4)}(\xi_1) + f^{(4)}(\xi_2)]h^4
\end{aligned}
$$

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

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

$$\frac{1}{2}[f^{(4)}(\xi_1) + f^{(4)}(\xi_2)] = f^{(4)}(\xi) \text{ for some } \xi \in (x_0 - h, x_0 + h)$$

Thus

$$f''(x_0) = \frac{f(x_0 + h) - 2f(x_0) + f(x_0 - h)}{h^2} - \frac{h^2}{12} f^{(4)}(\xi)$$

Error associated to computation derivative

$$f'(a) = \underbrace{\frac{f(a+h)-f(a-h)}{2h}}_{\text{approximation}} \quad + \underbrace{\frac{-h^2}{6}f^{(3)}(\xi)}_{\text{Error (discretization Error)}}$$

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 significant digits and there is loss of accuracy because of this.

$$f(x) = e^x \text{ and } a = 0$$

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

Analysis of this Phenomena

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

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

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

$$\text{So} \quad \underset{\text{Exact}}{\underset{\uparrow}{f'(a)}} = \underset{\text{Approximate}}{\underset{\uparrow}{f'_{comp}}} \; - \underset{\text{increases as } h \to 0}{\underset{\uparrow}{\frac{E_+ + E_-}{2h}}} \; - \underset{\text{decreases as } h \to 0}{\underset{\uparrow}{\frac{h^2 f^{(3)}(\xi)}{6}}}$$

Thus Numerical differentiation is an unstable process.

How to improve accuracy of computing derivatives

Use Richardson Extrapolation.

$$f'(a) = \frac{f(a+h) - f(a-h)}{h} + k_1 h + k_2 h^2 + \cdots + k_n h^n + \cdots$$

h sufficiently 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 sufficiently small k_i constant

Example

$$f(x) = sinx + cosx \text{ and } a = 0.3$$

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

Computation with 6 sig digits

h	$N_1(h)$	$N_2(h)$	$N_3(h)$	$N_4(h)$
0.1	$6.58717E{-1}$			
0.05	$6.59541E{-1}$	$6.59816E{-1}$		
0.025	$6.59748E{-1}$	$6.59817E{-1}$	$6.59817E{-1}$	
0.0125	$6.89799E{-1}$	$6.59816E{-1}$	$6.59816E{-1}$	$6.59816E{-1}$

Exact upto 6 sig digits

$$f'(0.3) = cos0.3 - sin0.3 = 6.59816E{-1}$$

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 linear Boundary-value problems in O.D.E.

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

$$y(a) = \alpha, \text{ and } y(b) = \beta, \; x \in [a, b]$$

$$h = \frac{b-a}{N}, \; x_0 = a, x_i = x_0 + ih, \text{ for } i = 1, \cdots, N$$

We use Central Difference approximation

$$y(x_i) = y_i \text{ , for } i = 1, 2, \cdots, N-1$$

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

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

Multiply 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

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

for every $i = 1, 2, \cdots, N-1$ as y_0 and y_N are known. This is an $(N-1) \times (N-1)$ system.

$$A \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N-1} \end{bmatrix} = b$$

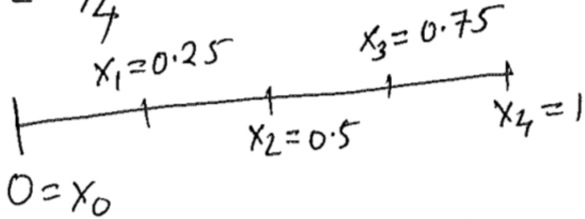
A is a tridiagonal matrix, $i.e.$ entries in the diagonal and above diagonal and below diagonal entries only.

Example

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

$$y(0) = 0, \; y(1) = 1$$

$h = 1/4$



Approximate y_1, y_2, y_3 and compare with exact solution $y(x) = \frac{sinx}{sin1}$

Solution

$$\frac{y_0 - 2y_1 + y_2}{h^2} + y_1 = 0, \quad \text{when } i = 1 \tag{3}$$

$$\frac{y_1 - 2y_2 + y_3}{h^2} + y_2 = 0, \quad \text{when } i = 2 \tag{4}$$

$$\frac{y_2 - 2y_3 + y_4}{h^2} + y_3 = 0, \quad \text{when } i = 3 \tag{5}$$

$$y_0 = 0, \;\; y_4 = 1$$

multiply equations (3),(4),(5) by h^2 and rearrange

$$
\begin{aligned}
(-2+h^2)y_1 + y_2 + 0y_3 &= 0\\
y_1 + (-2+h^2)y_2 + y_3 &= 0\\
0y_1 + y_2 + (-2+h^2)y_3 &= -1\\
-2+h^2 = -1.9375
\end{aligned}
$$

In six sig digits	exact $y(x) = \frac{sinx}{sin1}$
$y_1 = 2.94274E-1$	$y_1 = 2.94014E-1$
$y_2 = 5.70156E-1$	$y_2 = 5.69747E-1$
$y_3 = 8.10403E-1$	$y_3 = 8.10056E-1$

Our answers are correct upto 3 sig digits.

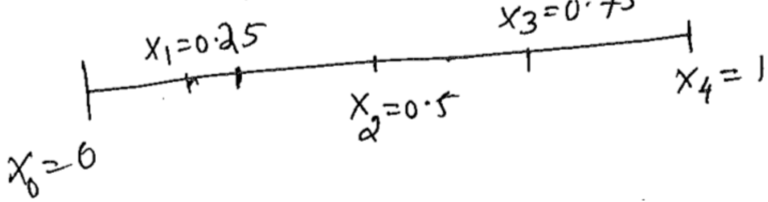
Exercise

Solve

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

$$y(0) = 0, \;\; y(1) = 1$$

$h = 1/4$



Approximate y_1, y_2, y_3 and compare with exact solution $y(x) = \frac{1}{1-e^{-1}}(1 - e^{-x})$

Solution

$$\begin{aligned}
\frac{y_0 - 2y_1 + y_2}{h^2} + \frac{y_2 - y_0}{2h} &= 0 \text{ , when } i = 1 & (6)\\
\frac{y_1 - 2y_2 + y_3}{h^2} + \frac{y_3 - y_1}{2h} &= 0 \text{ , when } i = 2 & (7)\\
\frac{y_2 - 2y_3 + y_4}{h^2} + \frac{y_4 - y_2}{2h} &= 0 \text{ , when } i = 3 & (8)
\end{aligned}$$

Multiply equations (6),(7),(8) by h^2 and rearrange. Also use $y_0 = 0, \; y_4 = 1$

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

$$h = 0.25, \ \frac{h}{2} = 0.125$$

Computed	exact $y(x) = \frac{1}{1-e^{-1}}(1-e^{-x})$
$y_1 = 3.50481E{-1}$	$y_1 = 3.49932E{-1}$
$y_2 = 6.23077E{-1}$	$y_2 = 6.22459E{-1}$
$y_3 = 8.35096E{-1}$	$y_3 = 8.34704E{-1}$

Not a 3 digit accuracy. So we have to take h smaller.

Remark:-

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

If we take h too small 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 $O(h^4)$ approximation.