Numerical Analysis : [MA214]
Lecture 7

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Recall

Last time we did improper integral

$$\int_a^b \frac{f(x)}{(x-a)^p} dx \text{ , } 0 < p < 1$$

with $f(x) \in C^4[a,b]$,
i.e., $f^{(4)}(x)$ exists and is continuous in $[a,b]$.
Let

$$\begin{aligned} P_4(x) &= f(a) + f'(a)(x-a) + \frac{f''(a)}{2}(x-a)^2 \\ &+ \frac{f^{(3)}(a)}{6}(x-a)^3 + \frac{f^{(4)}(a)}{24}(x-a)^4 \end{aligned}$$

be the 4^{th} Taylor polynomial of f around a

$$I = \int_a^b \frac{f(x)}{(x-a)^p} dx = \int_a^b \frac{f(x) - P_4(x)}{(x-a)^p} dx + \int_a^b \frac{P_4(x)}{(x-a)^p} dx$$

put

$$I_1 = \int_a^b \frac{P_4(x)}{(x-a)^p} dx$$

$$I_2 = \int_a^b \frac{f(x) - P_4(x)}{(x-a)^p} dx$$

I_1 will usually be the "dominant" part of I

$$G(x) = \left\{ \begin{array}{ll} \frac{f(x)-P_4(x)}{(x-a)^p} & \text{if } a < x < b \\ 0 & \text{if } x = a \end{array} \right\}$$

Then $G(x) \in C^4[a, b]$.

So we can use Simpson's Rule to approximate $I_2 = \int_a^b G(x)dx$.

Integrals of the form $\int_a^b \frac{f(x)}{(x-a)^p} dx$
($i.e.$ singularity at the right end point) can be converted into the previous form by change in variable $t = -x$.

if $a > 0$

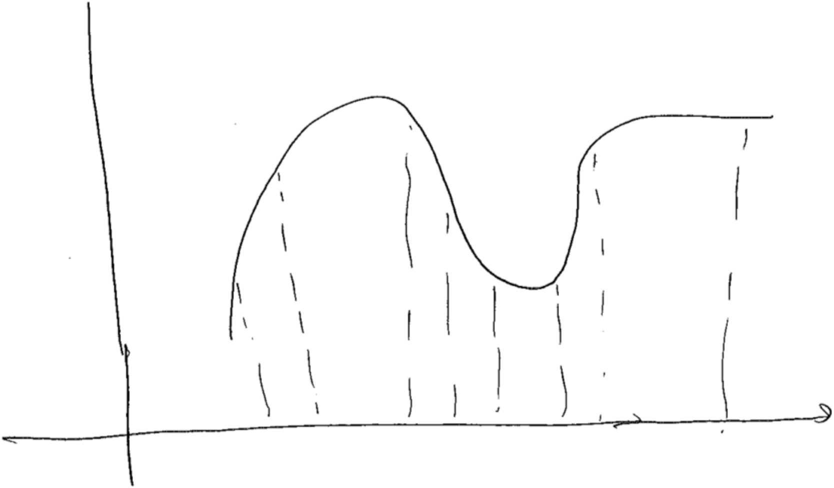
$$\int_a^\infty f(x)dx = \int_{\frac{1}{a}}^0 \frac{-1}{t^2} f(\frac{1}{t})dt$$

$$t = \frac{1}{x}, \text{ so } dt = -\frac{1}{x^2}dx = -t^2 dx$$

$$I = \int_a^\infty f(x)dx = \int_0^{\frac{1}{a}} t^{-2} f(\frac{1}{t})dt$$

is improper of the first kind.

Basic Idea of Adaptive Quadrature



Use more subdivisions when function is varying a lot.

Use fewer subdivisions when function is not changing much.

Question:- How to determine such intervals?

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

Need an approximation P to I such that

$$|P - I| < \epsilon \ (\ \epsilon = TOLERANCE \ )$$

Strategy for Adaptive Quadrature

First divide the interval $[a, b]$ into N subintervals
Usually $h = \frac{b-a}{N} \approx 0.5$

$$I_i = \int_{x_i}^{x_{i+1}} f(x)dx$$

We need approximation A_i such that

$$|I_i - A_i| \leq \epsilon \frac{b-a}{N}$$

$S_i =$ Simpson's rule applied to approximate I_i with step size $= h$.

$\overline{S_i} =$ Simpson's rule applied to approximate I_i with step size $= \frac{h}{2}$. and if each of these subintervals we arrange that the error estimate satisfies

$$|I_i - \overline{S_i}| \approx \frac{1}{15}|\overline{S_i} - S_i|$$

$|\overline{S_i} - S_i|$ can be computed.

$\overline{S_i}$ = approximate to I_i, if

$$\frac{1}{15}|\overline{S_i} - S_i| < \frac{b-a}{N}\epsilon$$

Otherwise $[x_i, x_{i+1}]$ is subdivided into two intervals and the entire process repeated.

Today we do Richardson Extrapolation

Extrapolation $\longleftrightarrow$ Using two lower order approximation to obtain higher order approximation.

This concept was invented by Richardson in 1927.

It was first used for weather forecasting.

Extrapolation can be applied whenever it is known that an approximation technique has an error term with a predictable form, one that depends on a "step size" h.

Assumption:-

For each $h \neq 0$ we have a formula $N(h)$ which approximate an unknown value M and the truncation error has the form

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

for some collection of unknown constant $k_1, k_2, k_3, \cdots$.

$$M \approx N(h) \text{ , is an } O(h) \text{ approximation}$$

Goal:- Combine $O(h)$ approximations to produce formulas with higher truncation error.

Method

$$M = N(h) + k_1 h + k_2 h^2 + k_3 h^3 + \cdots \tag{1}$$

This formula holds for all h (sufficiently small)

$$\lim_{h \to 0} N(h) = M$$

Set $N_1(h) = N(h)$

$$M = N(h/2) + k_1 \frac{h}{2} + k_2 \frac{h^2}{4} + k_3 \frac{h^3}{8} + \cdots \tag{2}$$

$2 \times (2) - (1)$ gives

$$M = 2N(h/2) - N(h) + k_2(\frac{h^2}{2} - h^2) + k_3(\frac{h^3}{4} - h^3)$$

$$M = \{N(h/2) + N(h/2) - N(h)\} + k_2' h^2 + k_3' h^3 + \cdots$$

Set

$$N_2(h) = N_1(h) + N_1(h/2) - N_1(h)$$

This is an $O(h^2)$ approximation.
Note: $k_2', k_3', \cdots$ are constants.

$$M = N_2(h) + k_2' h^2 + k_3' h^3 + \cdots \tag{3}$$

We replace h by $\frac{h}{2}$ in the formula (3)

$$M = N_2(h/2) + k_2' \frac{h^2}{4} + k_3' \frac{h^3}{8} + \cdots \tag{4}$$

$4 \times (4) - (3)$ gives

$$\begin{aligned} 3M &= 4N_2(h/2) - N_2(h) + k_3'' h^3 + k_4'' h^4 + \cdots \\ M &= N_2(h/2) + \frac{N_2(h/2) - N_2(h)}{3} + k_3'' h^3 + k_4'' h^4 + \cdots \end{aligned}$$

Set $N_3(h) = N_2(h/2) + \frac{N_2(h/2) - N_2(h)}{3}$

$$M = N_3(h) + k_3'' h^3 + k_4'' h^4 + \cdots$$

This is an order h^3 formula for approximating M.

Similarly

$$N_4(h) = N_3(h/2) + \frac{N_3(h/2) - N_3(h)}{7}$$

will be an $O(h^4)$ approximation to M

Table:-

In general

$$N_j(h) = N_{j-1}(h/2) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{2^{j-1} - 1}$$

h	$N_1(h)$			
$h/2$	$N_1(h/2)$	$N_2(h)$		
$h/4$	$N_1(h/4)$	$N_2(h/2)$	$N_3(h)$	
$h/8$	$N_1(h/8)$	$N_2(h/4)$	$N_3(h/2)$	$N_4(h)$

Example 1

$$e = \lim_{h \to 0} (1+h)^{1/h}$$

$$N(h) = (1+h)^{1/h}$$

One can show

$$e = N(h) + k_1 h + k_2 h^2$$

(All computations in 6 sig digits)

h	$N_1(h)$	$N_2(h)$	$N_3(h)$	$N_4(h)$
0.4	2.31910			
0.2	2.48832	2.65754		
0.1	2.59374	2.69916	2.71303	
0.05	2.65330	2.71286	2.71743	2.71806

Exact value of $e = 2.71828$ upto 6 sig digits.

Example 2

$$f(x) = sinx \ , \ x_0 = 0.2$$

$$f'(0.2) = \frac{f(0.2+h) - f(0.2)}{h} + k_1 h + k_2 h^2 + k_3 h^3 + \cdots$$

$$N(h) = \frac{f(0.2+h) - f(0.2)}{h}$$

h	$N(h)$	$N_1(h)$	$N_2(h)$
0.1	$9.685E{-1}$		
0.05	$9.747E{-1}$	$9.809E{-1}$	
0.025	$9.775E{-1}$	$9.803E{-1}$	$9.801E{-1}$

$cos(0.2) = 9.801E{-1}$, (correct upto 4 sig digits) .

Some time we have the following

$$M = N(h) + k_2 h^2 + k_4 h^4 + k_6 h^6 + \cdots \tag{5}$$

$N(h)$ is $O(h^2)$ approximation to M. Set $N_1(h) = N(h)$

Since equation (5) is valid for all h (sufficiently small) We have

$$M = N(h/2) + k_2 \frac{h^2}{4} + k_4 \frac{h^4}{16} + \cdots \tag{6}$$

$4 \times (6) - (5)$ gives

$$3M = 4N_1(h/2) - N_1(h) + k_4\left(\frac{h^4}{4} - h^4\right) + \cdots$$

$$M = N_1(h/2) + \frac{N_1(h/2) - N_1(h)}{3} + k_4' h^4 + k_6' h^6 + \cdots$$

Set

$$N_2(h) = N_1(h/2) + \frac{N_1(h/2) - N_1(h)}{3}$$

This is an $O(h^4)$ approximation.

$$M = N_2(h) + k_4' h^4 + k_6' h^6 + \cdots \tag{7}$$

We replace h by $\frac{h}{2}$ in equation (7) we get

$$M = N_2(h/2) + k_4' \frac{h^4}{16} + k_6' \frac{h^6}{64} + \cdots \tag{8}$$

$16 \times (8) - (7)$ gives

$$\begin{aligned} 15M &= 16N_2(h/2) - N_2(h) + k_6'(\frac{h^6}{4} - h^6) + \cdots \\ M &= N_2(h/2) + \frac{N_2(h/2) - N_2(h)}{15} + k_6'' h^6 + k_8'' h^8 + \cdots \end{aligned}$$

Set $N_3(h) = N_2(h/2) + \frac{N_2(h/2) - N_2(h)}{15}$
This is an h^6 approximation to M.

Continuing this way we get

$$N_j(h) = N_{j-1}(h/2) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{4^{j-1} - 1}$$

is $O(h^{2j})$ approximation to M

Example 3

$$e = \lim_{h \to 0} \left(\frac{2+h}{2-h} \right)^{1/h}$$

One can prove that

$$e = \left(\frac{2+h}{2-h} \right)^{1/h} + k_2 h^2 + k_4 h^4 + k_6 h^6 + \cdots + k_{2n} h^{2n} + \cdots$$

$$N_1(h) = \left(\frac{2+h}{2-h} \right)^{1/h}$$

(All computations in 8 sig digits)

h	$N_1(h)$	$N_2(h)$	$N_3(h)$	$N_4(h)$
0.4	2.7556760			
0.2	2.7274128	2.7179917		
0.1	2.7205514	2.7182643	2.7182825	
0.05	2.7188484	2.7182807	2.7182818	2.7182818

Our approximation $e = 2.7182818$ is correct upto 8 sig digits

Example 4

$$f(a+h) = f(a) + hf'(a) + \frac{h^2}{2!}f''(a) + \frac{h^3}{3!}f^{(3)}(a) + \cdots + \frac{h^n}{n!}f^{(n)}(a) + \cdots$$

$$f(a-h) = f(a) - hf'(a) + \frac{h^2}{2!}f''(a) - \frac{h^3}{3!}f^{(3)}(a) + \cdots + (-1)^n\frac{h^n}{n!}f^{(n)}(a) + \cdots$$

$$\frac{f(a+h) - f(a-h)}{2h} = f'(a) - k_2h^2 - k_4h^4 - \cdots$$

$$f'(a) = \frac{f(a+h) - f(a-h)}{2h} + k_2h^2 + k_4h^4 + \cdots$$

$f(x) = sinx$, $x_0 = 0.2$ (calculation in 8 sig digits)

h	$N(h)$	$N_1(h)$	$N_2(h)$	$N_3(h)$
0.1	$9.7843395E-1$			
0.05	$9.7965827E-1$	$9.8006638E-1$		
0.025	$9.7996449E-1$	$9.8006656E-1$	$9.8006657E-1$	
0.0125	$9.8004106E-1$	$9.8006658E-1$	$9.8006658E-1$	$9.8006658E-1$

$cos(0.2) = 9.8006658E-1$ correct upto 8 sig digits.

Extrapolation used in the context of composite Trapezoidal rule of integration is called Romberg integration.

Recall composite Trapezoidal rule

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

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

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

It can be shown that

$$I = T_N + c_1 h^2 + O(h^4)$$

$$c_1 = \frac{f'(a) - f'(b)}{12}$$

If N is even then note that one can use $T_{N/2}$ to compute T_N specifically

$$T_N = \frac{T_{N/2}}{2} + h\sum_{i=1}^{N/2} f(a + (2i-1)h)$$

One can prove that

$$I = T_N + c_2h^2 + c_4h^4 + c_6h^6 + \cdots + c_{2k}h^{2k} + \cdots$$

for all sufficiently small values of h $c_2, c_4, c_6, \cdots, c_{2k}, \cdots$ are constant independent of h.

$$T_N' = T_N + \frac{T_N - T_{N/2}}{3}$$

is $O(h^4)$ approximation to I.

$$I = T_N' + c_4'h^4 + c_6'h^6 + \cdots + c_{2k}'h^{2k} + \cdots$$

So one can do further extrapolation.

$$T_N^2 = T_N' + \frac{T_N' - T_{N/2}'}{15}$$

is $O(h^6)$ approximation to I.

More generally

$$T_N^m = T_N^{m-1} + \frac{T_N^{m-1} - T_{N/2}^{m-1}}{4^m - 1}$$

is $O(h^{2m+2})$ approximation to I.

Remark:- $\frac{N}{2^m}$ must be an integer for T_N^m to be defined.

Example 5

$$
\begin{aligned}
I &= \int_0^1 sin(x^2)dx \\
&= 0.3103 \text{ in 4 sig digits}
\end{aligned}
$$

(All computations in 4 sig digits)

N	T_N	T'_N	T^2_N	T^3_N
1	0.4208			
2	0.3341	0.3052		
4	0.3159	0.3098	0.3101	
8	0.3117	0.3103	0.3101	0.3103

Thus by Romberg integration we get accuracy upto 4 significant digits

Example 6

$$
\begin{aligned}
I &= \int_0^2 \sqrt{1 + cos^2 x} dx \\
&= 2.352 \text{ correct upto 4 sig digits}
\end{aligned}
$$

$$
\begin{aligned}
T_1 &= \frac{1}{2}.2[f(0) + f(1)] \\
&= 1[1.414 + 1.083] \\
&= 2.497
\end{aligned}
$$

$$
\begin{aligned}
T_2 &= \frac{1}{2}.1[f(0) + 2f(1) + f(2)] \\
&= \frac{1}{2}[2.497 + 1.137 \times 2] \\
&= \frac{1}{2}[4.771] = 2.386
\end{aligned}
$$

$$
\begin{aligned}
T_4 &= \frac{1}{2} 0.5[f(0) + 2f(0.5) + 2f(1) + 2f(1.5) + f(2)] \\
&= \frac{1}{4}[4.771 + 2f(0.5) + 2f(1.5)] \\
&= \frac{1}{4}[9.435] = 2.359
\end{aligned}
$$

Romberg Integration

N	T_N	T'_N	T^2_N	T^3_N
1	2.497			
2	2.386	2.349		
3	2.359	2.350	2.350	

So by Romberg integration error is reduced

Example 7

$$\begin{aligned} I &= \int_0^1 e^{-x^2}\,dx \\ \text{Find} &= T_1, T_2, T_4, T_8, \end{aligned}$$

and then complete the Romberg integration table.

$$\begin{aligned} T_1 &= \frac{1}{2}.1[f(0) + f(1)] \\ &= \frac{1}{2}[1 + 3.679E{-}1] \\ &= \frac{1}{2}[1.368] = 0.6840 \end{aligned}$$

$$
\begin{aligned}
T_2 &= \frac{1}{2}.\frac{1}{2}[f(0) + 2f(0.5) + f(1)] \\
&= \frac{1}{4}[1.368 + 2f(0.5)] \\
&= \frac{1}{4}[2.926] = 0.7314
\end{aligned}
$$

$$
\begin{aligned}
T_4 &= \frac{1}{2}\frac{1}{4}[f(0) + 2f(0.25) + 2f(0.5) + 2f(0.75) + f(1)] \\
&= \frac{1}{8}[2.926 + 2f(0.25) + 2f(0.75)] \\
&= \frac{1}{8}[5.944] = 0.7431
\end{aligned}
$$

$$
\begin{aligned}
T_8 &= \frac{1}{2}\frac{1}{8}[f(0) + 2f(0.125) + 2f(0.25) + 2f(0.375) + 2f(0.5) \\
&+ 2f(0.625) + 2f(0.75) + 2f(0.875) + f(1)] \\
&= \frac{1}{16}[5.944 + 2f(0.125) + 2f(0.375) + 2f(0.625) + 2f(0.875)] \\
&= \frac{1}{16}[11.93] = 0.7459
\end{aligned}
$$

Romberg Integration

N	T_N	T'_N	T^2_N	T^3_N
1	0.684			
2	0.7314	0.7472		
4	0.7431	0.7470	0.7470	
8	0.7459	0.7468	0.7468	0.7468

$$\int_0^1 e^{-x^2}\,dx = 0.7468$$

correct upto 4 sig digits.

Errors that occur under Richardson Extrapolation

1. If h is very small then we can have loss of significant digits. (This is not unique to Rechardson Extrapolation. It occurs in practically every numerical method)
2. Suppose

   $$M = N(h) + k_2 h^2 + k_4 h^4 + k_6 h^6 + \cdots$$

   for h " sufficiently small "

   Problem:- We do not know how small " sufficiently small" is.

Remark:- Even when these problems have been avoided we do not know how to get approximation. $|Exact - Approx| < Tol$

How to avoid problem associated with Richardson Extrapolation

Suppose

$$M = N(h) + k_2 h^2 + k_4 h^4 + k_6 h^6 + \cdots$$

So

$$\begin{aligned}
M &= N(h) + k_2 h^2 + O(h^4) \\
M &= N(2h) + k_2 4h^2 + O(h^4) \\
0 &= N(h) - N(2h) - 3k_2 h^2 + O(h^4) \\
k_2 h^2 &= \frac{N(h) - N(2h)}{3} + O(h^4) \\
k_2 h^2 &\approx \frac{N(h) - N(2h)}{3} \\
k_2 (h/2)^2 &\approx \frac{N(h/2) - N(h)}{3} \\
R_h^1 &= \frac{N(h) - N(2h)}{N(h/2) - N(h)} \approx \frac{k_2 h^2}{k_2 h^2/4} \approx 4
\end{aligned}$$

$$
\begin{aligned}
M &= N_2(h) + k_4 h^4 + O(h^6) \\
M &= N_2(2h) + k_4 16 h^4 + O(h^6) \\
0 &= N_2(h) - N_2(2h) - 15 k_4 h^4 + O(h^6) \\
k_4 h^4 &= \frac{N_2(h) - N_2(2h)}{15} + O(h^6) \\
k_4 h^4 &\approx \frac{N_2(h) - N_2(2h)}{15} \\
k_4 (h/2)^4 &\approx \frac{N_2(h/2) - N_2(h)}{15} \\
R_h^2 &= \frac{N_2(h) - N_2(2h)}{N_2(h/2) - N_2(h)} \approx \frac{k_4 h^4}{k_4 (h/2)^4} \approx 16
\end{aligned}
$$

In general

$$
R_h^k = \frac{N_k(h) - N_k(2h)}{N_k(h/2) - N_k(h)} \approx 4^k
$$

Example

$$e = \lim_{h \to 0} \left(\frac{2+h}{2-h} \right)^{1/h}$$

h	$N_1(h)$	R_h^1	$N_2(h)$	R_h^2
0.4	2.7556760			
0.2	2.7274128	4.12	2.7179917	
0.1	2.7205514	4.03	2.7182643	16.6
0.05	2.7188484	4.01	2.7182807	16.4
0.025	2.7184234	4.00	2.7182817	10
0.0125	2.7183172	4.01	2.7182818	1
0.00625	2.7182907	3.95	2.7182819	-1
$h_0 = 0.03125$	2.7182840	4.18	2.7182818	-1
$h_0/2$	2.7182824	4.00	2.7182819	$+\infty$
$h_0/4$	2.7182820	4.00	2.7182819	0

$h = 0.025$ gives best approximation.