Lecture 7

Last time we did improper integrals

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

with $f(x) \in C^4[a,b]$

i.e $f^{(iv)}(x)$ exists and is continuous in $[a,b]$.

Let $P_4(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2}(x-a)^2 + \frac{f'''(a)}{6}(x-a)^3 + \frac{f^{iv}(a)}{24}(x-a)^4$

be the 4th 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 $I_1 = \int_a^b \frac{P_4(x)}{(x-a)^p}\,dx$ $\quad I_2 = \int_a^b \frac{f(x) - P_4(x)}{(x-a)^p}\,dx$

I_1 will usually be the "dominant" part of I.

$$G(x) = \begin{cases} \dfrac{f(x) - P_4(x)}{(x-a)^p} & x \neq a \\ 0 & x = a \end{cases}$$

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

So we can use Simpsons' rule to approximate ~~$G(x)$~~. $I_2 = \int_a^b G(x)\,dx$.

Integrals of the form $\int_a^b \dfrac{f(x)}{(x-b)^p}\,dx$

(i.e singularity at the right-endpoint)

can be converted into the previous form by change in variable $t = -x$

---

if $a > 0$ $\quad \int_a^\infty f(x)\,dx = \int_{1/a}^0 f(t)\left(\frac{-1}{t^2}\right) dt$

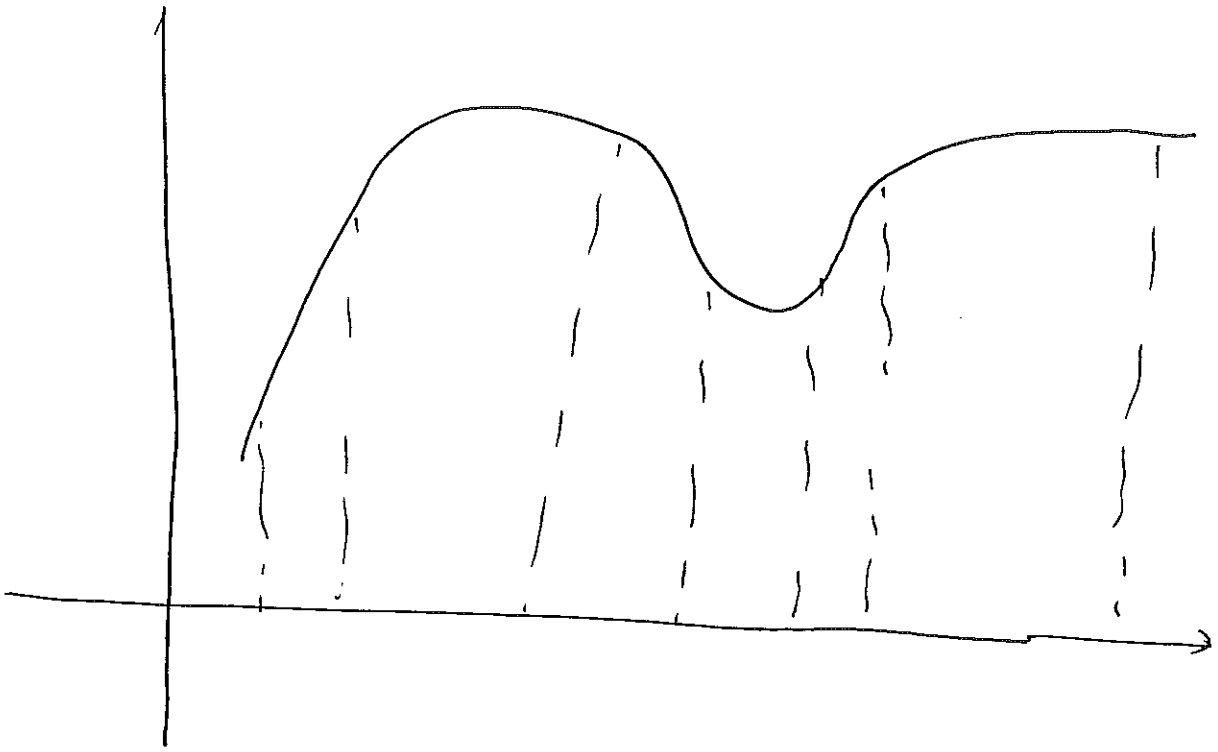
$$t = \frac{1}{x}$$

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

$I = \int_0^{1/a} f(1/t)\,\frac{1}{t^2}\,dt$ is improper of the first kind

Adaptive Quadrature

Basic idea of Adaptive Quadrature



Use more subdivisions when function is varying a lot

Use fewer subdivision when function is not changing much

Question :- How to determine such intervals?

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

Need approx s.t $|I - A| < \varepsilon$

ε = TOLERANCE

Strategy for adaptive Quadrature

first divide the interval $[a, b]$ into N sub-intervals

[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 s.t.

$$|I_i - A_i| \leq \varepsilon \cdot \frac{b-a}{N}.$$

S_i = Simpsons rule applied to approximate I_i with stepsize $= h$

$\bar{S}_i$ = " " " " approximate I_i with stepsize $h/2$

$$|I_i - \bar{S}_i| \approx \frac{1}{15} |S_i - \bar{S}_i|$$

↑ this can be computed

$\bar{S}_i$ = approximation to I_i if $\frac{1}{15}|S_i - \bar{S}_i| < \varepsilon \frac{b-a}{N}$.

Otherwise $[x_i, x_{i+1}]$ is subdivided into two intervals and 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 approximates 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 constants $K_1, K_2, K_3, \ldots$

$M \approx N(h)$ is an $O(h)$ approximation

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

Method

① $M = N(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots$

This formula holds for all h (sufficiently small)

$\lim_{h \to 0} N(h) = M$ set $N_1(h) = N(h)$

② $M = N(h/2) + K_1 h/2 + K_2 h^2/4 + K_3 h^3/8 + \cdots$

$2 \times$ ② − ① gives

$M = 2N(h/2) - N(h) + K_2 (h^2/2 - h^2) + K_3 (h^3/4 - h^3)$

③ $M = \{N(h/2) + N(h/2) - N(h)\} + K_2' h^2 + K_3' h^3 + \cdots$

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

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

Note K_2', K_3', ... are constants.

(3) $M = N_2(h) + K_2' h^2 + K_3' h^3 + \cdots$

We replace h by $h/2$ in formula (3)

(4) $M = N_2(h/2) + K_2' h^2/4 + K_3' h^3/8 + \cdots$

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

$3M = 4N_2(h/2) - N_2(h) + K_3'' h^3 + K_4''' h^4 + \cdots$

$M = N_2(h/2) + \dfrac{N_2(h/2) - N_2(h)}{3} + K_3'' h^3 + K_4''' h^4 + \cdots$

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

$M = N_3(h) + K_3'' h^3 + K_4'' h^4 + \cdots$

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

In general

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

will give $O(h^j)$ approximation to M

Table

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

$$e = N(h) + K_1 h + K_2 h^2 + \cdots$$

(all computations in 6 sig digit)

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 digit

Example 2

$$f(x) = \sin x$$

$$x_0 = 0.2$$

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

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

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

$\cos 0.2 = 9.801$ E-1 correct upto 4 sig digits

Sometimes we have the following

① $M = N(h) + K_2 h^2 + K_4 h^4 + K_6 h^6 + \cdots$

$N(h)$ is $O(h^2)$ approximation to M

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

Since ① is valid for all h (suff. small)

we have

② $M = N(h/2) + K_2 h^2/4 + K_4 h^4/16 + \cdots$

$4 \times ② - ①$ gives

$$3M = 4N_1(h/2) - N_1(h) + K_4(h^4/4 - h^4) + \cdots$$

$$M = N_1(h/2) + \frac{N_1(h/2) - N_1(h)}{3} + K_4' h^4 + K_6'' h^6$$

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

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

(3) $M = N_2(h) + K_4' h^4 + K_6' h^6 + \cdots$

replacing h by $h/2$ in (3) we get

$$M = N_2(h/2) + K_4' h^4/16 + K_6' h^6/64 + \cdots$$

$16 \times (4) - (3)$ yields

$$15M = 16 N_2(h/2) - N_2 h + K_6' (h^6/4 - h^6) + \cdots$$

$$M = N_2(h/2) + \frac{N_2(h/2) - N_2(h)}{15} + K_6'' h^6 + K_8'' h^8 + \cdots$$

$$N_3(h) = N_2(h/2) + \frac{N_2(h/2) - N_2(h)}{15}$$

This is an $O(h^6)$ 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

$$e = \left(\frac{2+h}{2-h} \right)^{1/h} + K_2 h^2 + K_4 h^4 + K_6 h^6 + \cdots + K_{2n} h^{2n} + \cdots$$

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

Calculations in 8 sig digits

h	N_1	N_2	N_3	N_4
0.4	2.75556760			
0.2	2.7274128	2.7179917		
0.1	2.7205514	2.7182643	2.7182825	
0.05	2.71888484	2.7182807	2.7182818	2.7182818

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

Example 4

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

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

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

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

calculation in 8 sig digits

$f(x) = \sin x \qquad a = 0.2$

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

$$\cos 0.2 = 9.8006658 \text{ E-1}$$

Romberg integration

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

Recall composite Trapezoidal rule

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

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

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

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

$$I = T_N + c_2 h^2 + c_4 h^4 + c_6 h^6 + \cdots + c_{2k} h^{2k} + \cdots$$

for all sufficiently small values of h

$c_2, c_4, c_6, \ldots, c_{2k}, \ldots$ are constants independent of h.

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

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

$$I = T_N^1 + C_4^1 h^4 + C_6^1 h^6 + \cdots + C_{2k}^1 h^{2k} + \cdots$$

So one can do further extrapolation.

$$T_N^2 = T_N^1 + \frac{T_N^1 - T_{N/2}^1}{15}$$

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 $N/2^m$ must be an integer for T_N^m to be defined.

Example 5

$$I = \int_0^1 \sin(x^2)\,dx$$

$$= 0.3103 \quad \text{in 4 sig digits}$$

(calc. in 4 sig digits)

N	T_N	T_N^1	T_N^2	T_N^3
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

$$I = \int_0^2 \sqrt{1+\cos^2 x}\, dx$$

$= 2.352$ (correct upto 4 sig. digits)

$$T_1 = \frac{1}{2} \cdot 2 \left[f(0) + f(1) \right]$$

$$= 1 \left[1.414 + 1.083 \right]$$

$$= 2.497$$

$$T_2 = \frac{1}{2} \cdot 1 \left[f(0) + 2f(1) + f(2) \right]$$

$$= \frac{1}{2} \left[2.497 + 1.137 \times 2 \right]$$

$$= \frac{1}{2} \left[4.771 \right]$$

$$= 2.386$$

$$T_4 = \frac{1}{2} 0.5 \left[f(0) + 2f(0.5) + 2f(1) + 2f(1.5) + f(2) \right]$$

$$= \frac{1}{4} \left[4.771 + 2f(0.5) + 2f(1.5) \right]$$

$$= \frac{1}{4} \left[9.435 \right] = 2.359$$

Romberg integration

N	T_N	T_N'	T_N''	T_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

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

Find T_1, T_2, T_4, T_8 and then complete the Romberg integration table.

$$T_1 = \frac{1}{2}.1\ (f(0) + f(1))$$

$$= \frac{1}{2}\ (1 + 3.679\ E{-}1)$$

$$= \frac{1}{2}\ (1.368)$$

$$= 0.6840$$

$$T_2 = \frac{1}{2}\ \frac{1}{2}\ (f(0) + 2f(0.5) + f(1))$$

$$= \frac{1}{4}\ (1.368 + 2f(0.5))$$

$$= \frac{1}{4}\ (2.926)$$

$$= 0.7314$$

$$T_4 = \frac{1}{2}\ \frac{1}{4}\ \Big[\begin{matrix} f(0) + 2f(0.25) + 2f(0.5) \\ +2f(0.75) + f(1) \end{matrix}\Big]$$

$$= \frac{1}{8}\ [2.926 + 2f(0.25) + 2f(0.75)]$$

$$= \frac{1}{8}\ [5.944]$$

$$= 0.7431$$

$$T_8 = \frac{1}{2}\cdot\frac{1}{8}\left\{\begin{array}{l} f(0)+2f(0.125)+2f(0.25) \\ +2f(0.375)+2f(0.5)+2f(0.625) \\ +2f(0.75)+2f(0.875)+f(1) \end{array}\right\}$$ (23)

$$= \frac{1}{16}\left\{5.944 + 2f(0.125)+2f(0.375) + 2f(0.625)+2f(0.875)\right\}$$

$$= \frac{1}{16}\{11.93\} = 0.7459$$

Rombery integration table

N	T_N	T_N^1	T_N^2	T_N^3
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

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

1) 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 approximations

$$|\text{Exact} - \text{Approx}| < \text{Tol}$$

How to avoid problems associated with Richardson Extrapolation

Suppose $M = N(h) + K_2 h^2 + K_4 h^4 + \cdots + K_{2k} h^{2k} + \cdots$

So $M = N(h) + K_2 h^2 + O(h^4)$

$M = N(2h) + K_2 4h^2 + O(h^4)$

$0 = N(h) - N(2h) - 3K_2 h^2 + O(h^4)$

$K_2 h^2 = \frac{N(h) - N(2h)}{3} + O(h^4)$

$K_2 h^2 \approx \frac{N(h) - N(2h)}{3}$

$K_2 (h/2)^2 \approx \frac{N(h/2) - N(h)}{3}$

$R_h = \frac{N(h) - N(2h)}{N(h/2) - N(h)} \approx \frac{K_2 h^2}{K_2 h^2/4} \approx 4$

$$M = N_2(h) + K_4 h^4 + O(h^6)$$

$$M = N_2(2h) + K_4 16 h^4 + O(h^6)$$

$$0 = N_2(h) - N_2(2h) - 15 h^4 K_4 + O(h^6)$$

$$K_4 h^4 = \frac{N_2(h) - N_2(2h)}{15} + O(h^6)$$

$$K_4 h^4 \approx \frac{N_2(h) - N_2(2h)}{15}$$

$$K_4 \left(\frac{h}{2}\right)^4 \approx \frac{N_2(h/2) - N_2(h)}{15}$$

$$R_h^2 = \frac{N_2(h) - N_2(2h)}{N_2(h/2) - N_2(h)} \approx \frac{K_4 h^4}{K_4 (h/2)^4} \approx 16$$

* 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			
			2.7179917	~~16.6~~
0.2	2.7274128	4.12		
			2.7182643	16.6
0.1	2.7205514	4.03		
			2.7182807	16.4
0.05 ~~0.05~~	2.7188484	4.01		
			2.7182817	10
0.025	2.7184234	4.00		
			2.7182818	1
0.0125	2.7183172	4.01		
			2.7182819	-1
0.00625	2.7182907	3.95		
			2.7182818	-1
h_0=0.003125	2.7182840	4.18		
			2.7182819	$+\infty$
$h_0/2$	2.7182824	4.00		
			2.7182819	0
$h_0/4$	2.7182820	4.00		
			2.7182819	
$h_0/8$	2.7182819			