3

Numerical Integration

Numerical integration is a tool used by engineers and scientists to definite integrals that cannot be solved analytically. In the area of statistical thermodynamics, the Debye model for calculating the heat capacity of a solid involves the integral :

$$I=\int_0^5 \frac{t^3}{e^t-1}dt \qquad (3.1)$$

As there is no exact solution for the integral (3.1), a numerical procedure may be used to obtain approximate solution by using the following standard methods :

Trapezoidal Rule

The approximation to integral :

$$I=\int_a^b f(x)dx \qquad (3.2)$$

may be obtained if f(x) is replaced by a suitable function that can easily be evaluated.

Suppose a function f(x) is known at equally spaced points in the interval [a,b] with step size h=(b-a)/N. N is a positive integer :

$$\left.\begin{matrix} x: x_0\ x_1\ \ldots\ x_{N-1}\ x_N \\ f: f_0\ f_1\ \ldots\ f_{N-1}\ f_N \end{matrix}\right\},\quad x_r = x_0 + rh,\ r = 0,1,2,\ldots,N$$

for which the integral (3.2) can be written as :

$$I = \int_a^b f(x)dx = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \ldots\ldots\ldots + \int_{x_{N-1}}^{x_N} f(x)dx \tag{3.3}$$

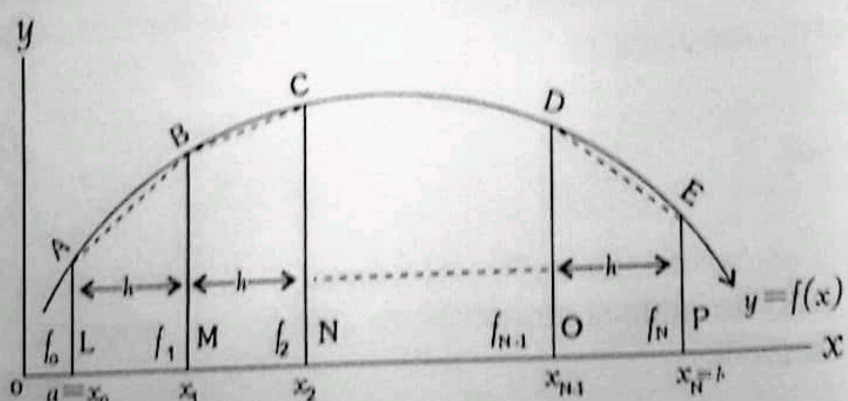

Fig 3.1: The Area of a Trapezia

1 : In interval [a,b] the area under the curve f(x) is approximated by the area of the **trapezia**; ABLM, BCMN,......,DEOP. For this, the sum of the integrals (3.3) can be written :

Area = [area of: ABLM + area of: BCMN + ... + area of: DEOP]

as an approximation I_h to I in the form :

$$\begin{aligned} I_h &= \frac{h}{2}(f_o+f_1)+\frac{h}{2}(f_1+f_2)+\dots\dots\dots+\frac{h}{2}(f_{N-1}+f_N) \\ &= h\left(\frac{1}{2}f_o+f_1+f_2+f_3+\dots\dots\dots+f_{N-1}+\frac{1}{2}f_N\right) \end{aligned} \quad (3.4)$$

is called **Trapezoidal rule** of numerical integration. The subscript h on I indicates the approximation to I depends on h.

2 : Another simplest method of approximation is obtained by replacing f(x) by a first degree interpolating polynomial $P_1(x)$ in the given interval [a,b]. For example, in subinterval $[x_o, x_1]$ the replacement of f(x) by $p_1(x)$ is giving linear interpolation through the points $(x_o, f_o), (x_1, f_1)$:

$$\int_{x_o}^{x_1} f(x)dx \approx \int_{x_o}^{x_1} p_1^{(o)}(x)dx = h\int_o^1 p_1^{(o)}(x_o+th)dt = h\int_o^1 (f_o+t\Delta f_o)dt = \frac{h}{2}(f_o+f_1)$$

This is the result previously obtained as the area of a trapezium **ABLM**.

Example 01 : *[trapezoidal rule]* : Approximate the integral :

$$I=\int_o^5 \frac{t^3}{e^t-1}dt, \quad 0 \le t \le 5$$

in the interval [0, 5] with step size h=1 for the tabulated data :

t	1	2	3	4	5
$t^3/(e^t-1)$	0.5819767	1.1763426	2.5522185	3.8770542	4.8998922

Trapezoidal rule (3.4) for the following assumptions :

$$\left.\begin{array}{l} h=1, t_1=1, t_2=2, \ldots\ldots, t_5=5, f(t)=t^3/(e^t-1) \\ f_1=0.5819767, f_2=1.1763426, \ldots\ldots, f_5=4.8998922 \end{array}\right\}$$ is used to obtain :

$$I_1=h\left(\frac{f_o}{2}+f_1+f_2+f_3+f_4+\frac{f_5}{2}\right)=4.8998922$$

Error Estimation and Correction

1 : Let $E_1^{(r)}$ be the truncation error developed in the Trapezoidal approximation over the interval $[x_r, x_{r+1}]$. Here the subscript 1 and the superscript r indicates that the function f(x) has been approximated by a first degree interpolating polynomial $P_1(x)$ in the interval $[x_r, x_{r+1}]$.

The local truncation error in the interval $[x_o, x_1]$:

$$E_1^{(o)}=\int_{x_o}^{x_1} f(x)dx-\int_{x_o}^{x_1} P_1^{(o)}(x)dx=\int_{x_o}^{x_1}[f(x)-P_1^{(o)}(x)]dx$$

that by putting $x=x_o+th$ becomes :

$$E_1^{(o)}=h\int_o^1\left[f(x_o+th)-\{f_o+t(f_1-f_o)\}\right]dt \qquad (3.5)$$

The expression in bracket can be expanded by Taylor series to obtain the truncation error in $P_1(x)$ by truncating the series after $O(h^2)$:

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$$E_1^{(o)}=h\int_o^1 \frac{t(t-1)h^2}{2!}f''(x_o)\,dt=-\frac{h^3}{12}f''(x_o) \quad \text{(consult chapter 2)}$$

It may be shown using a more rigorous analysis that :

$$E_1^{(o)}=\frac{-h^3}{12}f''(\eta_o),\ \ when\ \ x_o<\eta_o<x_1$$

The local truncation error for the typical interval $[x_r,x_{r+1}]$ is :

$$E_1^{(r)}=\frac{-h^3}{12}f''(\eta_r),\ \ when\ \ x_r<\eta_r<x_{r+1},\quad r=0,1,2,\ldots,N-1 \tag{3.6}$$

2 : If the only error at each step is that given by equation (3.6), then after N steps the accumulated error would be of order $O(h^2)$:

$$\begin{aligned} E&=-\sum_{r=o}^{N-1}\frac{h^3}{12}f''(\eta_r)=-\frac{Nh^3}{12}f''(\eta)=-\frac{(b-a/h)h^3}{12}f''(\eta),\ a<\eta<b \\ &=\left[-\frac{(b-a)}{12}f''(\eta)\right]h^2=Ch^2=O(h^2)\end{aligned} \tag{3.7}$$

3 : The global discretisation error is the difference of the exact and computed solutions. The error at the end point of the interval is called the **final global error (FGE) :**

$$E(I(b),h)=|I(b)-I_N|=O(h^2) \tag{3.8}$$

For example, if approximations are computed using the step sizes h, h/2 ,h/4,..., then :

$$E(I(b),h)\approx Ch^2 \quad \text{for the step size h} \tag{3.9}$$

$$E(I(b),h/2)\approx C\frac{h^2}{4}=\frac{1}{4}Ch^2=\frac{1}{4}E(I(b),h) \quad \text{for the step size h/2} \tag{3.10}$$

Hence the idea developed is that if the step size in Trapezoidal rule is reduced by a factor of 1/2, then the overall FGE will be reduced by a factor of 1/4.

Example 02 : ***[trapezoidal rule]*** : Approximate the integral :

$$I=\int_{o}^{1} e^{-x}dx$$

with h=1.0,0.5,0.25 and 0.125 for which the exact solution is 0.6321205588. Find also the upper and lower bounds for the accumulated error in this computation.

Trapezoidal rule (3.4) for the specified step sizes is used to obtain :

$$\begin{aligned}
I_1 &= (h/2)[f_o+f_1] = 0.683940, && h=1, && N=1\\
I_{o.5} &= (h/2)[f_o+2f_1+f_2] = 0.645235, && h=0.5, && N=2\\
I_{o.25} &= (h/2)[f_o+2f_1+2f_2+2f_3+f_4] = 0.635410, && h=0.25, && N=4\\
I_{o.125} &= (h/2)[f_o+2f_1+2f_2+2f_3+2f_4+2f_5+2f_6+2f_7+2f_8]\\
&= 0.632943, \quad h=0.125, \quad N=8
\end{aligned}$$

The accumulated error (3.7) for interval of width h is given by :

$$\left.\begin{aligned}
E &= -\frac{(b-a)h^2}{12}f^{II}(\eta), && a<\eta<b\\
|E| &= \frac{h^2}{12}e^{-\eta}, && o<\eta<1
\end{aligned}\right\}$$

If $f(x)=e^{-x}$ for $0<x<1$, then $e^{-1}<|f^{II}(x)|<e^{o}$.

Hence the lower and upper bounds for the accumulated error would also be of order $O(h^2)$:

$$\frac{h^2}{12}e^{-1} < |E| < \frac{h^2}{12}e^{o}$$

$$\left.\begin{array}{lll} For\ h=1 & 0.03066 < |E| < 0.08333 \\ For\ h=0.5 & 0.00766 < |E| < 0.02083 \\ For\ h=0.25 & 0.00192 < |E| < 0.00521 \\ For\ h=0.125 & 0.00048 < |E| < 0.00130 \end{array}\right\} \qquad (3.11)$$

Note that halving h reduces the error by a factor of 1/4.

EXAMPLE 02 THROUGH PACKAGE MMFP, COMPUTER PROGRAM 3-01: TRAPEZ
INPUT LIMITS A, B AND NUMBER OF SUBINTERVALS: 0.0 1.0 10
A=0.00, B=1.00, 10
THE COMPUTED SOL AT X=1.00 WITH 10 SUBINTERVALS
IS=0.6326472382D+00
THE EXACT SOL AT X=1.00 IS=0.6321205588D+00
THE FGE: AT A SPECIFIED POINT IS=0.5266793587D-03

Table 3.1 : Trapezoidal Approximations of Example 02 at a Fixed Point $x=1$ by a Package MMFP, Computer-Program 3-01: TRAPEZ.

Step Size: h	Intervals: N	Computed Sol: I_N	FGE
1.0	1	0.6839397206D+00	0.5181916176D-01
0.5	2	0.6452351901D+00	0.1311463132D-01
0.25	4	0.6354094290D+00	0.3288870199D-02
0.125	8	0.6329434182D+00	0.8228593819D-03

Note that halving h reduces the error by a factor of 1/4 and the overall FGE is nearly equal to the error noted in (3.11).

Simpson's Rule

An improvement in accuracy will be achieved, if the first degree interpolating polynomial $P_1(x)$ is replaced by a second degree interpolating polynomial $P_2(x)$ which fits f(x) at three consecutive points.

In this case, the function f(x) is known at equally even spaced points in the interval [a,b] with step size h=(b-a)/2N :

$$\left.\begin{matrix} x: x_o\ x_1\ x_2 \ldots\ x_{2N-2}\ x_{2N-1}\ x_{2N} \\ f: f_o\ f_1\ f_2 \ldots\ f_{2N-2}\ f_{2N-1}\ f_{2N} \end{matrix}\right\}, \quad x_{2r}=x_o+2rh,\ r=0,1,2,\ldots,N$$

for which the integral (3.2) can be written as :

$$I=\int_{x_0}^{x_2} f(x)dx+\int_{x_2}^{x_4} f(x)dx+\ldots+\int_{x_{2N-2}}^{x_{2N}} f(x)dx \quad (see\ fig{:}3.1) \tag{3.12}$$

The replacement of f(x) by a second degree interpolating polynomial $p_2^{(o)}(x)$ in subinterval $[x_o,x_2]$ is giving the quadratic interpolation through the points $(x_o,f_o),(x_1,f_1),(x_2,f_2)$:

$$\begin{aligned}\int_{x_o}^{x_2} f(x)dx &\approx \int_{x_o}^{x_2} p_2^{(o)}(x)dx=h\int_0^2 p_2^{(o)}(x_o+th)dt=h\int_0^2 [\,f_o+t\Delta f_o+\frac{t(t-1)}{2!}\Delta^2 f_o]dt \\ &=h\left| f_o t+t^2\Delta f_o/2+((t^3/6)-(t^2/4))\Delta^2 f_o\right|_o^2 \\ &= h\left(2f_o+2\Delta f_o+\frac{1}{3}\Delta^2 f_o\right) \\ &=h\left[2f_o+2(f_1-f_o)+\frac{1}{3}(f_2-2f_1+f_o)\right] \\ &=\frac{h}{3}(f_o+4f_1+f_2)\end{aligned} \tag{3.13}$$

This procedure for each even subinterval is continued till it reaches the approximate value of a function f(x) in the last subinterval $[x_{2N-2}, x_{2N}]$

The sum of the approximated values in each even subinterval denoted by I_h:

$$I_h = \frac{h}{3}\left[(f_o+4f_1+f_2)+(f_2+4f_3+f_4)+\ldots\ldots+(f_{2N-2}+4f_{2N-1}+f_{2N})\right]$$
$$=\frac{h}{3}\left[f_o+f_{2N}+4(f_1+f_3+\ldots\ldots+f_{2N-1})+2(f_2+f_4+\ldots\ldots+f_{2N-2})\right] \qquad (3.14)$$

is known as **Simpson's rule** of numerical integration.

Error Estimation and Correction

1 : The local truncation error for the typical interval $[x_{2r}, x_{2r+2}]$ can be found by expanding the terms in bracket by Taylor series to obtain :

$$E_2^{(r)} = \int_{x_{2r}}^{x_{2r+2}} [f(x)-p_2^{(r)}(x)]dx = \frac{-h^5}{90} f^{iv}(\eta_r), \text{ where } x_{2r}<\eta_r<x_{2r+2} \qquad (3.15)$$

2 : After N steps the accumulated error would be of order $O(h^4)$:

$$E = -\sum_{r=0}^{N-1} \frac{h^5}{90} f^{iv}(\eta_r) \approx -\frac{Nh^5}{90} f^{iv}(\eta), \quad a<\eta<b$$
$$= -\frac{((b-a)/2h)h^5}{90} f^{iv}(\eta), \text{ where } a<\eta<b \qquad (3.16)$$
$$= \left[-\frac{(b-a)f^{iv}(\eta)}{180}\right] h^4 = Ch^4 \approx O(h^4)$$

3 : The global discretisation error is the difference of the exact and computed solutions. The error at the end point of the interval is called the **final global error (FGE) :**

$$E(I(b),h) = |I(b) - I_N| = O(h^4) \tag{3.17}$$

For example, if approximations are computed using the step sizes h, h/2 ,h/4,…,then :

$$E(I(b),h) \approx Ch^4 \quad \text{for the step size h} \tag{3.18}$$

$$E(I(b),h/2) \approx C\frac{h^4}{16} = \frac{1}{16}Ch^4 = \frac{1}{16}E(I(b),h) \quad \text{for the step size h/2} \tag{3.19}$$

Hence the idea developed is that if the step size in Simpson's rule is reduced by a factor of 1/2, then the overall FGE will be reduced by a factor of 1/16.

Example 03 : *[simpson's rule]* : Approximate the integral :

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

with h=0.5,0.25 and h=0.125 for which the exact value is 0.6321205588. Find also the upper and lower bounds for the accumulated error in this computation.

Simpson's rule (3.14) for the specified step sizes is used to obtain :

$$I_{0.5} = \frac{h}{3}[f_o + 4f_1 + f_2] = 0.632334, \qquad h=0.5, \quad N=1$$

$$I_{o.25} = \frac{h}{3}[f_o + 4(f_1 + f_3) + 2f_2 + f_4] = 0.632134, \qquad h=0.25, \quad N=2$$

$$I_{0.125} = \frac{h}{3}[f_o + f_8 + 4(f_1 + f_3 + f_5 + f_7) + 2(f_2 + f_4 + f_6)] = 0.632121, \quad h=0.125, \quad N=4$$

The accumulated error (3.16) for interval of width h is given by :

$$\left.\begin{array}{ll} E=[-h^4/180]\ (b-a)f^{iv}(\eta), & a<\eta<b \\ |E|=\dfrac{h^4}{180}e^{-\eta}, & o<\eta<1 \end{array}\right\}$$

If $f(x)=e^{-x}$ for $o<x<1$, then $e^{-1}<|f^{iv}(x)|<e^{o}$.

Hence the lower and upper bounds for the accumulated error would also be of order $O(h^4)$:

$$\frac{h^4}{180}e^{-1} < |E| < \frac{h^4}{180}e^{0}$$

$$\left.\begin{array}{lllll} For\ h=0.5 & 0.00012774 & < & |E| & < 0.0003472 \\ For\ h=0.25 & 0.00000792 & < & |E| & < 0.0000217 \\ For\ h=0.125 & 0.00000049 & < & |E| & < 0.0000013 \end{array}\right\} \quad (3.20)$$

Note that halving h reduces the error by a factor of 1/16.

EXAMPLE 03 THROUGH PACKAGE MMFP, COMPUTER PROGRAM 3-02: SIMPSON
INPUT LIMITS A, B AND NUMBER OF SUBINTERVALS: 0.0 1.0 4
A=0.00, B=1.00, 10
THE COMPUTED SOL AT X=1.00 WITH 4 SUBINTERVALS
IS=0.6321214146D+00
THE EXACT SOL AT X=1.00 IS=0.6321205588D+00
THE FGE: AT A SPECIFIED POINT IS=0.8557761846D-06

Table 3.2 : Simpson's Approximations of Example 03 at a Fixed Point x=1 by a Package MMFP, Computer Program 3-02: SIMPSON.

Step Size: h	Intervals: N	Computed Sol: I_N	FGE
0.5	1	0.6323336800D+00	0.2131211751D-03
0.25	2	0.6321341753D+00	0.1361649197D-04
0.125	4	0.6321214146D+00	0.8557761846D-06

Note that halving h reduces the error by a factor of 1/16 and the overall

FGE is nearly equal to the error noted in equation (3.20).

Example 04 : For what values of h and N the **Trapezoidal** and **Simpson's** approximations of the integral :

$I=\int_{1.0}^{2.5} e^{x}dx$ are correct to 0.5×10^{-5}?

1 : The accumulated error in Trapezoidal rule for interval of width h is given by :

$$\left.\begin{aligned} E&=-\frac{h^2}{12}(b-a)f''(\eta), \quad a<\eta<b \\ |E|&=1.5\frac{h^2}{12}e^{\eta}, \quad 1.0<\eta<2.5 \end{aligned}\right\}$$

If $f(x)=e^x$ for $1.0<x<2.5$, then $e^{1.0}<|f''(x)|<e^{2.5}$. Hence :

$$[1.5h^2/12]e^{1.0}<|E|<[1.5h^2/12]e^{2.5}$$

To get an accuracy of 0.5×10^{-4} for the smallst value of h, let the upper bound should be :

$$\left.\begin{aligned} &\frac{1.5h^2}{12}e^{2.5}\leq0.5\times10^{-4} \\ &h^2\leq\frac{0.5\times10^{-4}}{1.522811745}=0.000032833 \\ &h=(0.000032833)^{1/2}=0.0057 \end{aligned}\right\} \quad N=\frac{(b-a)}{h}=\frac{1.5}{0.0057}=263$$

For 0.5×10^{-4} accuracy, the Trapezoidal rule requires 263 subintervals with step size h=0.0057.

2 : The accumulated error in Simpson's rule for interval of width h is given by :

$$\left.\begin{aligned} E &= -\frac{h^4}{180}(b-a)f^{iv}(\eta), \quad a<\eta<b \\ |E| &= \frac{1.5h^4}{180}e^{\eta}, \qquad 1.0<\eta<2.5 \end{aligned}\right\}$$

For getting an accuracy of 0.5×10^{-4}, let the upper bound should be :

$$\left.\begin{aligned} &\frac{1.5h^4}{180}e^{2.5} \le 0.5\times10^{-4} \\ &h^4 \le \frac{0.5\times10^{-4}}{0.101520783} = .000492509 \\ &h \approx (0.000492509)^{1/4} = 0.149 \end{aligned}\right\} \quad N = \frac{(b-a)}{2h} = \frac{1.5}{0.298} = 5.033 \approx 6$$

For the same accuracy, the Simpson's rule requires 6 subintervals with step size h=0.149.

The technique which will be used, if one wishes to get a method of higher order, is the :

Romberg Integration

To give better approximation by considering $h\to0$: The technique of combining two approximated values obtained by using the same method with two different step sizes to get a higher order method is called the extrapolation method or **Richardson's extrapolation.** This process of combining approximations produced by Richardson's extrapolation is called **Romberg integration**.

Trapezoidal Extrapolation : If Trapezoidal approximations with different step sizes $h, h/2, h/4, h/8.$ to integral (3.2) are $I_h, I_{h/2}, I_{h/4}, I_{h/8}\ldots\ldots$

then the $O(h^4)$ **extrapolations** for which :

a : I_h and $I_{h/2}$ may be combined by Richardson's extrapolation to get $I_{h,h/2}$, which has an error of the form $C_4 h^4$. C_4 is constant.

b : $I_h/2$ and $I_{h/4}$ may be combined to get $I_{h/2,h/4}$, which has an error of the form $C_4^* h^4$. C_4^* is constant.

c : $I_{h/4}$ and $I_{h/8}$ may be combined to get $I_{h/4,h/8}$, which has an error of the form $C_4^{**} h^4$. C_4^{**} is constant.

For above results, let the truncation error in Trapezoidal rule for small h can be represented as :

$$E = E(h) = E_2 h^2 + E_4 h^4 + E_6 h^6 + \ldots, \quad E_2, E_4, E_6, \ldots \text{ are constants} \tag{3.21}$$

The error equation (3.21) is substituted in the integral (3.2) for the different step sizes h, h/2, h/4, h/8 to obtain :

$$\begin{aligned}
I &= I_h + E = I_h + E_2 h^2 + E_4 h^4 + E_6 h^6 + \ldots\ldots (i) \\
I &= I_{h/2} + E = I_{h/2} + E_2 (h/2)^2 + E_4 (h/2)^4 + E_6 (h/2)^6 + \ldots\ldots (ii) \\
I &= I_{h/4} + E = I_{h/4} + E_2 (h/4)^2 + E_4 (h/4)^4 + E_6 (h/4)^6 + \ldots\ldots (iii) \\
I &= I_{h/8} + E = I_{h/8} + E_2 (h/8)^2 + E_4 (h/8)^4 + E_6 (h/8)^6 + \ldots\ldots (iv)
\end{aligned} \tag{3.22}$$

For $I_{h,h/2}$, eliminating E_2 from the above Eqs:(i) & (ii) to obtain :

$$\left.\begin{aligned} 4I-I &= 4I_{h/2}-I_h - (3/4)E_4h^4 - (15/16)E_6h^6-.....\\ I &= \frac{1}{3}\left[4I_{h/2}-I_h\right] - (1/4)E_4h^4 - (5/16)\,E_6h^6-..... \end{aligned}\right\} 4(ii)-(i) \tag{3.23}$$

$$\text{where } I_{h,h/2} = \frac{1}{3}\left[4I_{h/2}-I_h\right]=I_T^1(h)$$

For $I_{h/2,h/4}$, eliminating E_2 from the above Eqs:(ii) & (iii) to obtain :

$$\left.\begin{aligned} 4I-I &= 4I_{h/4}-I_{h/2} -(3/64)E_4h^4-(15/1024)E_6h^6-.......\\ I &= \frac{1}{3}\left[4I_{h/4}-I_{h/2}\right]-(1/64)E_4h^4-(5/1024)\,E_6h^6-....... \end{aligned}\right\} 4(iii)-(ii) \tag{3.24}$$

$$\text{where } I_{h/2,h/4}=\frac{1}{3}[4I_{h/4}-I_{h/2}]=I_T^1(h/2)$$

For $I_{h/4,h/8}$, eliminating E_2 from the above Eqs:(iii) & (iv) to obtain :

$$\left. I=\frac{1}{3}\left[4I_{h/8}-I_{h/4}\right]-(1/1024)E_4h^4-(5/65536)E_6h^6-.......\right\} 4(iv)-(iii) \tag{3.25}$$

$$\text{where } I_{h/4,h/8}=\frac{1}{3}\left[4I_{h/8}-I_{h/4}\right]=I_T^1(h/4)$$

The methods (3.23), (3.24) and (3.25) will be used to approximate the integral (3.2) with truncation errors :

$$\left.\begin{aligned} (-1/4)E_4h^4 &= C_4h^4\\ (-1/64)E_4h^4 &= C_4^*h^4\\ (-1/1024)E_4h^4 &= C_4^{**}h^4 \end{aligned}\right\} \text{ which are of } O(h^4).$$

For $O(h^6)$ **extrapolations :**

d : $I_{h,h/2}$ and $I_{h/2,h/4}$ may be combined to obtain $I_{h,h/2,h/4}$, which has an error of the form $C_6 h^6$. C_6 is constant.

e : $I_{h/2,h/4}$ and $I_{h/4,h/8}$ may be combined to obtain $I_{h/2,h/4,h/8}$, whic

has an error of the form $C_6^* h^6$. C_6^* is constant.

For $I_{h,h/2,h/4}$, eliminating E_4 from $O(h^4)$ methods (3.23) and (3.24) b

subtracting {16(3.24)-(3.23)} to obtain :

$$\left.\begin{aligned} 16I-I &= \frac{16}{3}(4I_{h/4}-I_{h/2})-\frac{1}{3}(4I_{h/2}-I_h)+(15/64)E_6h^6+\ldots\ldots \\ I &= \frac{1}{15}\left[\frac{16}{3}(4I_{h/4}-I_{h/2})-\frac{1}{3}(4I_{h/2}-I_h)\right]+(1/64)\,E_6h^6+\ldots\ldots \end{aligned}\right\} \quad (3.2$$

$$\text{where } I_{h,h/2,h/4}=\frac{1}{15}\left[\frac{16}{3}(4I_{h/4}-I_{h/2})-\frac{1}{3}(4I_{h/2}-I_h)\right]=I_T^2(h)$$

For $I_{h/2,h/4,h/8}$, eliminating E_4 from $O(h^4)$ methods (3.24) and (3.

by subtracting {16(3.25)-(3.24)} to obtain :

$$\left.I_{h/2,h/4,h/8}=\frac{1}{15}\left[\frac{16}{3}(4I_{h/8}-I_{h/4})-\frac{1}{3}(4I_{h/4}-I_{h/2})\right]+(1/4096)E_6h^6+\ldots\ldots\right\} \quad (3.$$

$$\text{where } I_{h/2,h/4,h/8}=\frac{1}{15}\left[\frac{16}{3}(4I_{h/8}-I_{h/4})-\frac{1}{3}(4I_{h/4}-I_{h/2})\right]=I_T^2(h/2).$$

The methods (3.26) and (3.27) will be used to approximate the inte (3.2) with truncation errors :

$$\left.\begin{aligned} (1/64)E_6h^6 &= C_6h^6 \\ (1/4096)E_6h^6 &= C_6^*h^6 \end{aligned}\right\} \text{ which are of order } O(h^6).$$

This procedure of combining results is continued till it develops the higher order method of order **m** based on Trapezoidal rule :

$$I_T^m(h) = \frac{4^m I_T^{(m-1)}(h/2) - I_T^{(m-1)}(h)}{4^m - 1}, \quad m = 1, 2, \ldots \tag{3.28}$$

where $I_T^o(h) = I_h$, $I_T^o(h/2) = I_{h/2}$

This formula for various values of **m** is tabulated as under :

Extrapolation Table Based on Trapezoidal Rule

S.Size	$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$
h	I_h			
		$I_T^1(h)$		
$h/2$	$I_{h/2}$		$I_T^2(h)$	
		$I_T^1(h/2)$		$I_T^3(h)$
$h/4$	$I_{h/4}$		$I_T^2(h/2)$	
		$I_T^1(h/4)$		
$h/8$	$I_{h/8}$			

Example 05 : ***[romberg based on trapezoidal rule]*** : Approximate the integral :

$$I = \int_0^1 e^{-x} dx, \quad h = 1, 0.5, 0.25 \text{ to clarify :}$$

1 : How many subintervals will be required for the accuracy 0.1×10^{-5}, when the integral is approximated directly by **Trapezoidal** rule for which the exact solution is 0.6321205588 ?

2 : How many functions evaluations will be required for the same accuracy, when the integral is approximated by **Romberg** based on Trapezoidal ?

The $O(h^2)$ Trapezoidal approximations from table 3.1 :

$I_h = I_1 = 0.683939721$, $I_{h/2} = I_{0.5} = 0.645235190$, $I_{h/4} = I_{0.25} = 0.635409429$,
$I_{h/8} = I_{0.125} = 0.632943418$

are used in $O(h^4)$ method (3.28) to obtain :

$$I_{h,h/2} = I_T^1(h) = (1/3)[4I_{h/2} - I_h] = 0.632333680$$
$$I_{h/2,h/4} = I_T^1(h/2) = (1/3)[4I_{h/4} - I_{h/2}] = 0.632134175$$
$$I_{h/4,h/8} = I_T^1(h/4) = (1/3)[4I_{h/8} - I_{h/4}] = 0.632121414$$

that can be substituted in $O(h^6)$ method (3.28) to obtain :

$$I_{h,h/2,h/4} = I_T^2(h) = (1/15)[16I_T^1(h/2) - I_T^1(h)] = 0.632120874$$
$$I_{h/2,h/4,h/8} = I_T^2(h/2) = (1/15)[16I_T^1(h/4) - I_T^1(h/2)] = 0.632120563$$

Extrapolation Table Based on Trapezoidal Rule

S.Size	$O(h^2)$	$O(h^4)$	$O(h^6)$
h	0.683939721		
		0.632333680	
1/2	0.645235190		0.632120874
		0.632134175	
1/4	0.635409429		0.632120563
		0.632121414	
1/8	0.632943418		

Table 3.3 : FGE's of the Higher Order Methods obtained by Romberg Integration based on Trapezoidal Approximations of Example 05 at a Fixed Point x=1.

h	FGE: $O(h^2)$	FGE: $O(h^4)$	FGE: $O(h^6)$
1.0	0.051819610		
0.5	0.013114631	0.000213121	
0.25	0.003288870	0.000013616	0.000000315
0.125	0.000822859	0.000000855	0.000000004

Note that halving h reduces the error by a factors of **1/4**, **1/16** and 1/64.

Romberg integration based on Trapezoidal approximations consumes **four** extrapolations and **eight** functions evaluations to get an accuracy of

0.1×10^{-5}.

The accumulated error in Trapezoidal rule for interval of width h is given by :

$$\left.\begin{aligned} E &= \frac{-(b-a)h^2}{12} f^{II}(\eta), & a<\eta<b \\ |E| &= \frac{h^2}{12} e^{-\eta}, & o<\eta<1 \end{aligned}\right\}$$

If $f(x) = e^{-x}$ *for* $o<x<1$, then $e^{-1} < |f^{II}(x)| < e^{-o}$.

Hence the lower and upper bounds for the accumulated error would also be of order $O(h^2)$:

$$\frac{h^2}{12} e^{-1} < \left|\frac{h^2}{12} e^{-\eta}\right| < \frac{h^2}{12} e^{-0}$$

To get an accuracy of 0.1×10^{-5}, let the lower bound should be :

$$\left.\begin{aligned}\frac{h^2e^{-1}}{12} &\leq 0.1\times10^{-5}\\ h^2 &\leq \frac{10^{-6}}{0.0307}\\ h &\approx (0.000033)^{1/2}=0.006\end{aligned}\right\} \quad N=\frac{(b-a)}{h}=\frac{1}{0.006}=167$$

For the same accuracy, the Trapezoidal rule requires **167 subintervals** with step size **h=0.006.**

EXAMPLE 05 THROUGH PACKAGE MMFP, COMPUTER PROGRAM 3-03: ROMBERG
INPUT LIMITS A.B AND ERROR TOL: 0.0 1.0 .000001
A0.00, B=1.00, TOL=0.1000D-05
ROMBERG TABLE BASED ON TRAP RULE AFTER 3 EXTRAPOLATIONS :

0.6839397206D+00			
0.6452351901D+00	0.6323336800D+00		
0.6354094290D+00	0.6321341753D+00	0.6321208750D+00	
0.6329434182D+00	**0.6321214146D+00**	0.6321205639D+00	**0.6321205590D+00**

Simpson's Extrapolation : The truncation error in Simpson's rule can be written as

$$E=E_4h^4+E_6h^6+E_8h^8+\ldots\ldots \tag{3.29}$$

The error equation (3.29) is substituted in the integral (3.2) for the different step sizes h, h/2, h/4 to obtain :

$$\begin{aligned} I &= I_h+E=I_h+E_4h^4+E_6h^6+E_8h^8+\ldots\ldots(i)\\ I &= I_{h/2}+E=I_{h/2}+E_4(h/2)^4+E_6(h/2)^6+E_8(h/2)^8+\ldots\ldots(ii)\\ I &= I_{h/4}+E=I_{h/4}+E_4(h/4)^4+E_6(h/4)^6+E_8(h/4)^8+\ldots\ldots(iii)\end{aligned} \tag{3.30}$$

For $I_{h,h/2}$, eliminating E_4 from Eqs:(i) & (ii) to obtain :

$$\left.\begin{aligned} I &= \frac{1}{15}\left[16I_{h/2}-I_h\right]-\frac{1}{20}E_6h^6-\frac{1}{16}E_8h^8-\ldots\ldots \\ \text{where } I_{h,h/2} &= \frac{1}{15}\left[16I_{h/2}-I_h\right]=I_S^1(h) \end{aligned}\right\} \qquad (3.31)$$

For $I_{h/2,h/4}$, eliminating E_4 from Eqs:(ii) & (iii) to obtain

$$\left.\begin{aligned} I &= \frac{1}{15}\left[16I_{h/4}-I_{h/2}\right]-\frac{1}{1280}E_6h^6-\frac{1}{4096}E_8h^8-\ldots\ldots \\ \text{where } I_{h/2,h/4} &= \frac{1}{15}\left[16I_{h/4}-I_{h/2}\right]=I_S^1(h/2) \end{aligned}\right\} \qquad (3.32)$$

The methods (3.31) and (3.32) will be used to approximate the integral (3.2) with truncation errors :

$$\left.\begin{aligned} (-1/20)E_6h^6 &= C_6h^6 \\ (-1/1280)E_6h^6 &= C_6^*h^6 \end{aligned}\right\} \text{ which are of order } O(h^6).$$

For $O(h^8)$ extrapolation $I_{h,h/2,h/4}$, eliminating E_6 from $O(h^6)$ methods (3.31) and (3.32) to obtain :

$$\left.\begin{aligned} I &= \frac{1}{63}\left[\frac{64}{15}(16I_{h/4}-I_{h/2})-\frac{1}{15}(16I_{h/2}-I_h)\right]+\frac{1}{1344}E_8h^8+\ldots\ldots \\ \textbf{where } I_{h,h/2,h/4} &= \frac{1}{63}\left[\frac{64}{15}(16I_{h/4}-I_{h/2})-\frac{1}{15}(16I_{h/2}-I_h)\right]=I_S^2(h) \end{aligned}\right\} \qquad (3.33)$$

The method (3.33) will be used to approximate the integral (3.2) with truncation error $(1/1344)E_8h^8=C_8h^8$, which is of order $O(h^8)$.

This procedure of combining results is continued till it develops the higher order method of order **m** based on Simpson's rule :

$$I_S^m(h) = \frac{4^{m+1} I_S^{m-1}(h/2) - I_S^{m-1}(h)}{4^{m+1} - 1}, \quad m = 1, 2, \ldots \tag{3.34}$$

where $I_S^o(h) = I_h$, $I_S^o(h/2) = I_{h/2}$

This formula for various values of **m** is tabulated as under :

Extrapolation Table Based on Simpson's Rule

S.Size	$O(h^4)$	$O(h^6)$	$O(h^8)$
h	I_h		
		$I_S^1(h)$	
$h/2$	$I_{h/2}$		$I_S^2(h)$
		$I_S^1(h/2)$	
$h/4$	$I_{h/4}$		

Example 06 : ***[romberg based on simpson rule]*** : Approximate the integral :

$$I = \int_0^1 e^{-x} dx, \quad h = 0.5, 0.25, 0.125$$ to clarify :

1 : How many subintervals will be required for the 0.1×10^{-5} accuracy, when the integral is approximated directly by **Simpson's** rule for which the exact solution is 0.6321205588 ?

2 : How many functions evaluations will be required for the same accuracy, when the integral is approximated by **Romberg** based on Simpson ?

The $O(h^4)$ Simpson's approximations from table 3.2 :

$I_h = I_{0.5} = 0.63233680$, $I_{h/2} = I_{0.25} = 0.632134175$, $I_{h/4} = I_{0.125} = 0.632121415$

are used in $O(h^6)$ method (3.34) to obtain :

$$I_{h,h/2} = I_S^1(h) = (1/15)[16 I_{h/2} - I_h] = 0.632120666$$
$$I_{h/2,h/4} = I_S^1(h/2) = (1/15)[16 I_{h/4} - I_{h/2}] = 0.632120564$$

Extrapolation Table Based on Simpson's Rule

h	$O(h^4)$	$O(h^6)$
0.5	0.63233680	
		0.632120666
0.25	0.632134175	
		0.632120564
0.125	0.632121415	

Romberg integration based on Simpson's approximations consumes **one** extrapolation and **four** functions evaluations to get an accuracy of 0.1×10^{-5}.

The accumulated error in Simpson's rule for interval of width h is given by :

$$\left.\begin{aligned} E &= \frac{-(b-a)h^4}{180} f^{iv}(\eta), && a<\eta<b \\ |E| &= \frac{h^4}{180} e^{-\eta}, && 0<\eta<1 \end{aligned}\right\}$$

If $f(x) = e^{-x}$ for $0 \le x \le 1$, then $e^{-1} \le |f^{iv}(x)| \le e^{-0}$.

Hence the lower and upper bounds for the accumulated error would also be of order $O(h^4)$:

$$\frac{h^4}{180}e^{-1} \le \left|\frac{h^4}{180}e^{-\eta}\right| \le \frac{h^4}{180}e^{o}$$

To get an accuracy of 0.1×10^{-5}, let the lower bound should be :

$$\frac{h^4e^{-1}}{180} \le 0.1\times10^{-5}$$

$$h^4 \le \frac{10^{-6}}{0.00204}$$

$$h \approx (0.000497)^{1/4} = 0.149$$

$$N = \frac{(1-0)}{0.298} = 3.36 \approx 4$$

For the same accuracy, the Simpson's rule consumes **four** subintervals with step size **h=0.149.**

Exercises : Chapter-3

1. For the following integrals :

$$i : \int_{o}^{4} x^2e^{-x}dx \qquad ii : \int_{1/4}^{4} \frac{1}{\sqrt{x}}dx$$

$$iii : \int_{-1}^{1} \frac{1}{1+x^2}dx \qquad iv : \int_{o}^{1} (2+\sin 2\sqrt{x})\,dx$$

use a package MMFP of computer programs 3-01,3-02,3-03 to:

a : Obtain the **Trapezoidal approximations** for N=10,20,30
b : Obtain the **Simpson approximations** for N=5,10,20
c : Obtain the **Romberg approximations** for the limits A,B with correction

tolerance 0.5×10^{-6}.

2. Approximate the integral :

$$I=\int_{1}^{6} 2+\sin(2\sqrt{x})dx$$

a : By Trapezoidal rule with N=5 and N=10
b : By Simpson's rule with N=5 and N=10
c : Use a package MMFP of computer programs 3-01,3-02 to check the results obtained by using (a) and (b).

3. **Length of a curve :** The arc length of the curve y=f(x) over the interval $a\le x\le b$ is

$$length=\int_{a}^{b}\sqrt{1+[f'(x)]^2}\,dx$$

Use the functions :

$$\left.\begin{array}{l} i:\ f(x)=x^3 \ for\ o\le x\le 1 \quad ii:\ f(x)=\sin x\ for\ o\le x\le \pi/4 \\ iii:\ f(x)=e^{-x}\ for\ o\le x\le 1 \end{array}\right\}\ to$$

a : Approximate the arc length using Trapezoidal rule with N=10.
b : Approximate the arc length using Simpson's rule with N=5.
c : Use a package MMFP of computer programs 3-01,3-02 to check the results obtained by using (a) and (b).

4. **Surface area :** The solid of revolution obtained by rotating the region under the curve y=f(x) over the interval $a\le x\le b$ about the x-axis has surface area given by :

$$A=2\pi\int_{a}^{b} f(x)\sqrt{1+[f'(x)]^2}\,dx$$

Use the functions in exercise 3 to :

a : Approximate the area using Trapezoidal rule with N=10.
b : Approximate the area using Simpson's rule with N=5.
c : Use a package MMFP of computer programs 3-01,3-02 to check the results obtained by using (a) and (b).

5. Use Romberg integration based on Trapezoidal rule to approximate the integral:

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

to obtain $O(h^4)$ extrapolation for the step sizes h=0.5, 0.25 with correction tolerance 0.5×10^{-6}.

6. Use Simpson's rule to approximate the integral :

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

for the step sizes h=0.5, 0.25. Combine these two results to obtain $O(h^6)$ Simpson's extrapolation with correction tolerance 0.5×10^{-6}. .

7. Use Romberg integration to approximate the integral :

$$I=\int_1^2 \frac{dx}{x}$$

Carry six decimals and continue until no change in the fifth place occurs. Compare to the actual value ln 2=0.69315.

8. Use Simpson's rule to approximate the integral :

$$I=\int_0^1 e^x dx$$

by choosing h small enough to guarantee five decimal accuracy. How large can h be ?

9. Show that the Simpson's approximation and the extrapolated approximations from two applications of the Trapezoidal rule for the integral available in exercise 8 are identical. Show that this will always be true.

10. Approximate the integral :

$I=\int_{0}^{1} \cos x\,dx$ by using

a : Romberg integration based on Trapezoidal rule with h=0.2, 0.1, 0.05.
b : Romberg integration based on Simpson's rule with h=0.2, 0.1, 0.05.
c : Use a package MMFP of computer programs 3-01,3-03 to check the results obtained by using (a) with correction tolerance 0.5×10^{-6}.

11. For what values of h the step size and N the number of sub intervals, the **Trapezoidal** approximation for the following integrals :

$a: \int_{2}^{7} dx/x \qquad b: \int_{2}^{3} dx/(5-x) \qquad c: \int_{0}^{2} xe^{-x}dx$

is correct to 0.5×10^{-5} ?

12. For what values of h the step size and 2N the number of sub intervals, the **Simpson's approximation** for the integrals available in exercise 11 is correct to 0.5×10^{-5} ?

13. Approximate the integral :

$I=\int_{0}^{1}\frac{dx}{1+x}$ to clarify :

a : How many subintervals will be required for the accuracy of 10^{-6}, when the integral is approximated directly by Trapezoidal rule ?
b : How many subintervals will be required for the same accuracy, when the integral is approximated directly by Simpson's rule ?

c : How many functions evaluations will be required for the same accuracy, when the integral is approximated by Romberg based on Trapezoidal rule with $h = 1.0, 0.5, 0.25, 0.125$?
d : How many functions evaluations will be required for the same accuracy, when the integral is approximated by Romberg based on Simpson's rule with $h = 0.5, 0.25, 0.125$?
e : Use a package MMFP of computer programs **3-01 TRAPEZ, 3-02 SIMPSON and 3-03 ROMBERG** to check the results obtained by using (a), (b) and (c).