Chapter 4

Numerical Differentiation and Integration

4.1 Numerical Differentiation:

Suppose $f \in C^2[a,b]$ and $x_0 \in [a,b]$ (an arbitrary point)

We are interested in an approx. to $f'(x_0)$.

Let $x_1 = x_0 + h$ $\quad h \neq 0$ (small such that $x_1 \in [a,b]$)

Using Theo. 3.3

$$f(x) = P(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^{n} (x - x_i)$$

$$\rightarrow f(x) = P_{0,1}(x) + \frac{(x-x_0)(x-x_1)}{2!} f''(\xi(x))$$

$$= \frac{f(x_0)[x-(x_0+h)]}{-[(x_0+h)-x_0]} + \frac{f(x_0+h)(x-x_0)}{[(x_0+h)-x_0]} + \frac{(x-x_0)[x-(x_0+h)]}{2} f''(\xi(x))$$

(P 133)

$\xi(x) \in [a,b]$

$$f'(x) = \frac{f(x_0+h) - f(x_0)}{h} + D_x\left[\frac{(x-x_0)(x-x_0-h)}{2} f''(\xi(x))\right]$$

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

$$+ \frac{(x-x_0)(x-x_0-h)}{2} D_x(f''(\xi(x)))$$

$$f'(x) \approx \frac{f(x_0+h) - f(x_0)}{h}$$

Difficulty: For arbitrary x, we have no information about $D_x f''(\xi(x)) = f'''(\xi(x)) \cdot \xi'(x)$ $\left(\begin{array}{l}\text{Remark:} \\ f \in C^2[a,b]\end{array}\right)$

(we want to find $f'(x_0)$ but we faced with f'' !)

But when $x = x_0 \rightarrow$ the coff. of $D_x f''(\xi(x)) = 0$

$$\rightarrow \quad f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} - \frac{h}{2} f''(\xi(x))$$

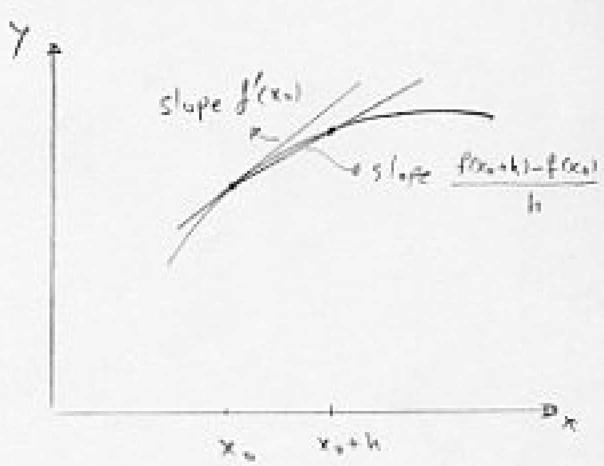
For h = small

$$f'(x_0) \simeq \frac{f(x_0+h) - f(x_0)}{h}$$

$$\text{Error bound} = M \frac{h}{2} \quad \left(\begin{array}{l} M \text{ a bound on } f''(x) \\ \text{for } x \in [a,b] \end{array}\right)$$

This formula is Known as $\begin{cases} \text{Forward difference formula} & \text{if } h > 0 \\ \text{Backward} \quad " \quad " & \text{if } h < 0 \end{cases}$

<u>Ex.</u>



$f(x) = \ln x \qquad x_0 = 1.8$

$$f'(1.8) \approx \frac{f(1.8+h) - f(1.8)}{h} \qquad h > 0$$

$$\text{Error} = \frac{|h f''(\xi)|}{2} = \frac{|h|}{2\xi^2} \leqslant \frac{|h|}{2(1.8)^2}$$

$1.8 < \xi < 1.8 + h$

$$\text{Error}_{max} = \frac{|h|}{2(1.8)^2}$$

h	$f(1.8+h)$	$\frac{f(1.8+h)-f(1.8)}{h}$	$\frac{\|h\|}{2(1.8)^2}$
0.1	0.64185389	0.5406722	0.154321
0.01	0.59332685	0.5540180	0.0015432
0.001	0.58834207	0.5554013	0.0001543

Since $f'(x) = \frac{1}{x} \longrightarrow f'(1.8) = 0.55\bar{5}$ (exact)

More General derivative approx. Formula

Suppose $\{x_0, x_1, \dots x_n\}$ are $(n+1)$ distinct numbers $\in (I)$

and $f \in C^{n+1}(I)$. $\quad$ I: some interval

Acc. to Theo. 3.3:

$$f(x) = \sum_{k=0}^{n} f(x_k) L_k(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^{n} (x - x_i)$$

$\xi(x) \in (I)$

$L_k(x)$: kth Lagrange coff. polynomial for f at $x_0, x_1 \dots x_n$

$$f'(x) = \sum_{k=0}^{n} f(x_k) L_k'(x) + D_x\left[\frac{\prod_{i=0}^{n}(x-x_i)}{(n+1)!}\right] f^{(n+1)}(\xi(x))$$

$$+ \frac{\prod_{i=0}^{n}(x-x_i)}{(n+1)!} D_x\left[f^{(n+1)}(\xi(x))\right]$$

Again; we have difficulty of estimating the truncation error, unless $X = X_k \quad k \in (0, 1, \ldots n)$

In this case, The term involving $D_x \left[f^{(n+1)}(\xi(x)) \right] = 0$

$$\rightarrow f'(x_k) = \sum_{j=0}^{n} f(x_j) L_j'(x_k) + \frac{f^{(n+1)}(\xi(x_k))}{(n+1)!} \prod_{\substack{j=0 \\ j \neq k}}^{n} (x_k - x_j) \qquad (1)$$

This is called $(n+1)$-point formula to approximate $f'(x_k)$.

Using more evaluation points $\longrightarrow$ $\begin{cases} \text{greater accuracy} \\ \text{but growth of rounding error} \end{cases}$

Most common formulas are $\begin{cases} \text{3-evaluation points} \\ \text{5- ″ ″} \end{cases}$

3 - Evaluation Points:

$$L_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} \quad \rightarrow L_0'(x) = \frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}$$

Similarly:

$$L_1'(x) = \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \quad \text{and} \quad L_2'(x) = \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}$$

From equ (1):

$$f'(x_j) = f(x_0) \left[\frac{2x_j - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} \right] + f(x_1) \left[\frac{2x_j - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \right]$$

$$+ f(x_2) \left[\frac{2x_j - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} \right] + \frac{1}{6} f^{(3)}(\xi_j) \prod_{\substack{i=0 \\ i \neq j}}^{2} (x_j - x_i)$$

$j = 0, 1, 2$

ξ_j indicates that this point depends on x_j.

This formula become specially useful if the nodes are <u>equally spaced</u>;

i.e. $x_1 = x_0 + h$, $x_2 = x_0 + 2h$ $\quad h \neq 0$

Using $x_j = x_0$, $x_1 = x_0 + h$, $x_2 = x_0 + 2h$

$$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2} f(x_0) + 2f(x_1) - \frac{1}{2} f(x_2)\right] + \frac{h^2}{3} f^{(3)}(\xi_0) \qquad (1)$$

Similarly if $x_j = x_1$

$$f'(x_1) = \frac{1}{h}\left[-\frac{1}{2} f(x_0) + \frac{1}{2} f(x_2)\right] - \frac{h^2}{6} f^{(3)}(\xi_1) \qquad (2)$$

and for $x_j = x_2$

$$f'(x_2) = \frac{1}{h}\left[\frac{1}{2} f(x_0) - 2f(x_1) + \frac{3}{2} f(x_2)\right] + \frac{h^2}{3} f^{(3)}(\xi_2) \qquad (3)$$

As a matter of convenience;

$x_0 + h \longrightarrow x_0$ in (2)

$x_0 + 2h \longrightarrow x_0$ " (3)

$$\rightarrow \quad f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_0) \qquad (4)$$

$$f'(x_0) = \frac{1}{2h}\left[-f(x_0-h) + f(x_0+h)\right] - \frac{h^2}{6} f^{(3)}(\xi_1) \qquad (5)$$

$$f'(x_0) = \frac{1}{2h}\left[f(x_0-2h) - 4f(x_0-h) + 3f(x_0)\right] + \frac{h^2}{3} f^{(3)}(\xi_2) \qquad (6)$$

Equ.(6) can be obtained from equ.(4) by simply replacing h with $-h$, then there are actually only two formulas:

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_0) \qquad (7)$$

where ξ_0 : between x_0 and x_0+2h

$$f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] - \frac{h^2}{6} f^{(3)}(\xi_1) \qquad (8)$$

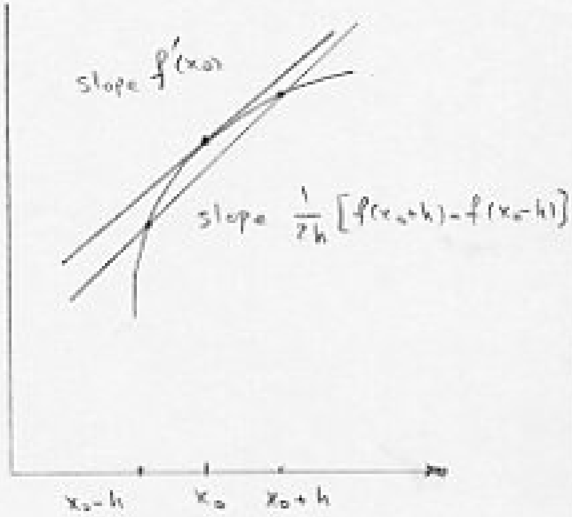
where ξ_1 : between (x_0-h) and (x_0+h)

The error of equ.(8) $= \frac{1}{2}$ error in equ(7)

This is reasonable; because in equ.(8) data is being exmined on <u>both</u> sides of x_0, but on only <u>one</u> side in equ(7).

Also; $\begin{cases} \text{In equ.(8), } f \text{ needs to be evaluated in } \underline{\text{two}} \text{ points} \\ \text{In " (7), } \underline{\text{three}} \text{ evaluations are needed.} \end{cases}$

Approx. of equ. (7) is useful at the ends of interval I.



Approximation of equ (8)

5-Points Formula:

$$f'(x_0) = \frac{1}{12h}\left[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h) \right] + \frac{h^4}{30} f^{(5)}(\xi) \quad (9)$$

Another one;

$$f'(x_0) = \frac{1}{12h}\left[-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h) + 16f(x_0+3h) - 3f(x_0+4h) \right] + \frac{h^4}{5} f^{(5)}(\xi) \quad (10)$$

ξ: between x_0 and x_0+4h

In left end point approx. ; $h>0$

In right " " " ; $h<0$

Ex.

Given in Table are values for $f(x) = xe^x$

$f'(x) = (x+1)e^x \qquad f'(2.0) = 22.167168$

x	f(x)
1.8	10.889365
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

3-point formulas:

Using (7),
$$\begin{cases} h = 0.1 & f'(2.0) \simeq \frac{1}{0.2}\left[-3f(2.0)+4f(2.1)-f(2.2)\right] = 22.032310 \\ h = -0.1 & f'(2.0) \simeq \frac{1}{-0.2}\left[-3f(2.0)+4f(1.9)-f(1.8)\right] = 22.054525 \end{cases}$$

Using (8),
$$\begin{cases} h = 0.1 & f'(2.0) \simeq \frac{1}{0.2}\left[f(2.1)-f(1.9)\right] = 22.228790 \\ h = 0.2 & f'(2.0) \simeq \frac{1}{0.4}\left[f(2.2)-f(1.8)\right] = 22.414163 \end{cases}$$

5-point formula:

Using (9):

$$h = 0.1 \qquad f'(2.0) \simeq \frac{1}{1.2}\left[f(1.8)-8f(1.9)+8f(2.1)-f(2.2)\right] = 22.166999$$

The errors respectively; $\begin{cases} 1.35\times 10^{-1} \\ 1.13\times 10^{-1} \\ -6.16\times 10^{-2} \\ -2.47\times 10^{-1} \\ 1.69\times 10^{-4} \end{cases}$ (approximately)

Higher Order Derivatives:

Expand $f(x)$ in a third Taylor polynomial about x_0 and evaluate at x_0+h and x_0-h

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

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

where $x_0-h < \xi_{-1} < x_0 < \xi_1 < x_0+h$

Adding them;

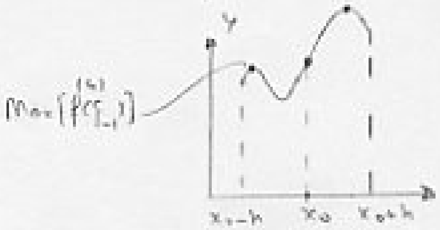
$$f(x_0+h) + f(x_0-h) = 2f(x_0) + f''(x_0)h^2 + \frac{1}{24}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})\right]h^4$$

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

If $f^{(4)} \in C[x_0-h, x_0+h]$, acc. to Intermediate Value Theo. (P55)

$$f''(x_0) = \frac{1}{h^2}\left[f(x_0-h) - 2f(x_0) + f(x_0+h)\right] - \frac{h^2}{12}f^{(4)}(\xi) \begin{cases} \mathrm{Max}(f^{(4)}(\xi_1)) \\ \mathrm{Max}(f^{(4)}(\xi_{-1})) \end{cases}$$

for some ξ, where $x_0 - h < \xi < x_0 + h$



Ex. Using the data for $f(x) = xe^x$ in the last example

we approximate $f''(2.0)$

$h=0.1$ $\quad f''(2.0) \approx \frac{1}{0.01}\left[f(1.9) - 2f(2.0) + f(2.1)\right] = 29.593200$

$h=0.2$ $\quad f''(2.0) \approx \frac{1}{0.04}\left[f(1.8) - 2f(2.0) + f(2.2)\right] = 29.704275$

Since $f''(x) = (x+2)e^x \longrightarrow f''(2.0) = 29.556224$

the errors are approximately, -3.70×10^{-2} and -1.48×10^{-1}, respectively.

The Effect of Round off Errors:

Let us examine;

$$f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h) \right] - \frac{h^2}{6} f^{(3)}(\xi_1)$$

Suppose; $e(x_0+h)$: rounding error of $f(x_0+h)$

$e(x_0-h)$: " " " $f(x_0-h)$

$\Rightarrow$

$$f(x_0+h) = \tilde{f}(x_0+h) + e(x_0+h)$$

$$f(x_0-h) = \tilde{f}(x_0-h) + e(x_0-h)$$

↑ true value ↑ computed value

$$f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} = \frac{e(x_0+h) - e(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi_1)$$

(total error)

If the rounding error is bounding by some $\epsilon > 0$

$$|e(x_0 \pm h)| \leq \epsilon$$

and also $|f^{(3)}| \leq M$ $(M > 0)$

$$\left| f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} \right| \leq \frac{\epsilon}{h} + \frac{h^2}{6} M$$

To reduce truncation error $\xrightarrow{\text{we must}}$ reduce h

But as h reduces $\longrightarrow$ roundoff error grows.

Ex.

Consider approximating $f'(0.900)$ for $f(x) = \sin x$ using the Table.

The true value is $f' = \cos(0.900) = 0.62161$
rad

Using the formula

$$f'(0.900) \simeq \frac{f(0.900+h) - f(0.900-h)}{2h} \qquad \text{(3-point formula)}$$

x	Sin x	x	Sin x
0.800	0.71736	0.901	0.78395
0.850	0.75128	0.902	0.78457
0.880	0.77074	0.905	0.78643
0.890	0.77707	0.910	0.78950
0.895	0.78021	0.920	0.79560
0.898	0.78208	0.950	0.81342
0.899	0.78270	1.000	0.84147

h	Approx. $f'(0.900)$	Error
0.001	0.62500	0.00339
0.002	0.62250	0.00089
0.005	0.62200	0.00039
0.010	0.62150	-0.00011
0.020	0.62150	-0.00011
0.050	0.62160	-0.00021
0.100	0.62055	-0.00106

optimal choice for h

$$e(h) = \frac{\epsilon}{h} + \frac{h^2}{6}M \qquad \frac{\partial e(h)}{\partial h} = 0 \longrightarrow h = \sqrt[3]{3\epsilon/M} \quad (\text{Min. of } e(h))$$

$$M = \max_{x \in [0.800,\, 1.00]} |f'''(x)| = \max_{x \in [0.800,\, 1.00]} |\cos x| \simeq 0.69671$$

Since the values of f are given to five decimal points

$\longrightarrow$ it is reasonable to assume that $\epsilon = 0.000005$

$$h = \sqrt[3]{\frac{3(0.000005)}{0.69671}} \simeq 0.028$$

However, we cannot compute an optimal h, since we have no Knowledge of $f'''(x)$ (in general we don't have the func. $f(x)$).

Numerical differentiation is unstable,

since $h \longrightarrow$ small $\longrightarrow \begin{cases} \text{reduces truncation error} \\ \text{causes the rounding error to grow.} \end{cases}$

4.3 Elements of Numerical Integration:

The basic method involved in approximating $\int_a^b f(x)\,dx$ is called numerical quadrature, an uses a sum of the type;

$$\sum_{i=0}^{n} a_i f(x_i)$$

to approximate $\int_a^b f(x)dx$

The methods of quadrature in this section are based on the interpolation polynomials given in chapter 3.

We select distinct nodes $\{x_0, x_1, \dots x_n\} \in [a,b]$

$$P_n(x) = \sum_{i=0}^{n} f(x_i)\, L_i(x) \qquad \text{Lagrange interpolating polynomial}$$

$$\int_a^b f(x)dx = \int_a^b \sum_{i=0}^{n} f(x_i) L_i(x) + \int_a^b \prod_{i=0}^{n} (x-x_i) \frac{f^{(n+1)}(\xi(x))}{(n+1)!} dx$$

$$= \sum_{i=0}^{n} a_i f(x_i) + \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^{n} (x-x_i) f^{(n+1)}(\xi(x)) dx$$

where $\xi(x) \in [a,b]$

and $a_i = \int_a^b L_i(x) dx \qquad i = 0, 1, \ldots n$

$$\int_a^b f(x)dx \simeq \sum_{i=0}^{n} a_i f(x_i) \qquad \text{quadrature formula}$$

$$E(f) = \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^{n} (x-x_i) f^{(n+1)}(\xi(x)) dx$$

Trapezoidal rule: (first Lagrange polynomials with equally spaced nodes)

let $x_0 = a \quad x_1 = b \qquad h = b - a$

$$P_1(x) = \frac{(x-x_1)}{(x_0-x_1)} f(x_0) + \frac{(x-x_0)}{(x_1-x_0)} f(x_1) \qquad \text{Linear Lagrange polynomial}$$

Thus:

$$\int_a^b f(x)dx = \int_{x_0}^{x_1} \left[\frac{(x-x_1)}{(x_0-x_1)} f(x_0) + \frac{(x-x_0)}{(x_1-x_0)} f(x_1) \right] dx$$

$$+ \frac{1}{2} \int_{x_0}^{x_1} f''(\xi(x))(x-x_0)(x-x_1) dx$$

Since $(x-x_0)(x-x_1)$ does not change sign on $[x_0, x_1]$, the Weighted Mean Value Theo. for Integrals can be applied to the error term; (P55)

$$\int_{x_0}^{x_1} f''(\xi(x))(x-x_0)(x-x_1)\,dx = f''(\xi)\int_{x_0}^{x_1}(x-x_0)(x-x_1)\,dx$$

$$= f''(\xi)\left[\frac{x^3}{3} - \frac{(x_1+x_0)}{2}x^2 + x_0 x_1 x\right]_{x_0}^{x_1} = -\frac{h^3}{6}f''(\xi)$$

$$\int_a^b f(x)\,dx = \left[\frac{(x-x_1)^2}{2(x_0-x_1)}f(x_0) + \frac{(x-x_0)^2}{2(x_1-x_0)}f(x_1)\right]_{x_0}^{x_1} - \frac{h^3}{12}f''(\xi)$$

$$= \frac{(x_1-x_0)}{2}\left[f(x_0)+f(x_1)\right] - \frac{h^3}{12}f''(\xi)$$

Since $h = x_1 - x_0$

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(x_0)+f(x_1)\right] - \frac{h^3}{12}f''(\xi) \quad \text{Trapezoidal Rule}$$

Trapazoidal Rule gives exact result if $f''(x) = 0$ (polynomial of deg ≤ 1)

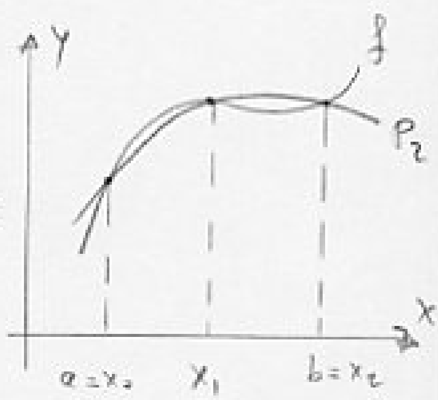
Trapezoidal Rule

Simpson's Rule : (Second Lagrange polynomial with nodes $x_0 = a$, $x_2 = b$, $x_1 = a+h$, where $h = \frac{b-a}{2}$)

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_2} \Big[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) +$$

$$+ \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \Big] dx$$

$$+ \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\xi(x))\,dx$$



Deriving Simpson's rule in this manner $\xrightarrow{\text{Provides}}$ $\begin{cases} O(h^4) \text{ error involving} \\ f^{(3)} \end{cases}$

Alternative approach $\xrightarrow{\text{results}}$ a higher order involving $f^{(4)}$

Consider third Taylor expansion about x_1,

For each $x \in [x_0, x_2]$ $\quad \exists\ \xi(x)$ in (x_0, x_2) with

$$f(x) = f(x_1) + f'(x_1)(x-x_1) + \frac{f''(x_1)}{2}(x-x_1)^2 + \frac{f'''(x_1)}{6}(x-x_1)^3 + \frac{f^{(4)}(\xi(x))}{24}(x-x_1)^4$$

$$\int_{x_0}^{x_2} f(x)\,dx = f(x_1)(x_2-x_0) + \Big[\frac{f'(x_1)}{2}(x-x_1)^2 + \frac{f''(x_1)}{6}(x-x_1)^3 + \frac{f'''(x_1)}{24}(x-x_1)^4 \Big]_{x_0}^{x_2} + \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x-x_1)^4\,dx$$

Since $(x-x_1)^4 > 0$ on $[x_0, x_2]$, the Weighted Mean Value Theo. for Integrals implies that:

(P55)

$$\frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x_1))(x-x_1)^4\,dx = \frac{f^{(4)}(\xi_1)}{24}\int_{x_0}^{x_2}(x-x_1)^4\,dx$$

$$= \frac{f^{(4)}(\xi_1)}{120}(x-x_1)^5\Big|_{x_0}^{x_2}$$

$\xi_1 \in (x_0, x_2)$

However: $h = x_2 - x_1 = x_1 - x_0$

$$\longrightarrow (x_2-x_1)^2-(x_0-x_1)^2 = (x_2-x_1)^4-(x_0-x_1)^4 = 0$$

$$(x_2-x_1)^3-(x_0-x_1)^3 = 2h^3$$

$$(x_2-x_1)^5-(x_0-x_1)^5 = 2h^5$$

$$\longrightarrow \int_{x_0}^{x_2} f(x)\,dx = 2h\,f(x_1) + \frac{h^3}{3}f''(x_1) + \frac{f^{(4)}(\xi_1)}{60}h^5$$

Using

$$f''(x_0) = \frac{1}{h^2}\left[f(x_0-h) - 2f(x_0) + f(x_0+h)\right] - \frac{h^2}{12}f^{(4)}(\xi) \quad \text{(P145)}$$

$$\int_{x_0}^{x_2} f(x)\,dx = 2h\,f(x_1) + \frac{h^3}{3}\left\{\frac{1}{h^2}\left[f(x_0) - 2f(x_1) + f(x_2)\right] - \frac{h^2}{12}f^{(4)}(\xi_2)\right\}$$

$$+ \frac{f^{(4)}(\xi_1)}{60}h^5$$

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}\left[f(x_0)+4f(x_1)+f(x_2)\right] - \frac{h^5}{12}\left[\frac{1}{3}f^{(4)}(\xi_2)-\frac{1}{5}f^{(4)}(\xi_1)\right]$$

It can be shown ξ_1 and ξ_2 can be replaced by a common ξ in (x_0,x_2)

$$\to \int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}\left[f(x_0)+4f(x_1)+f(x_2)\right] - \frac{h^5}{90}f^{(4)}(\xi)$$

Simpson's Rule

Error $= E(f^{(4)})$

Simpson's Rule gives exact result, if $f(x)$ is polynomial of deg ≤ 3.

Ex. The Trapezoidal rule for a func. $f(x)$ on the interval $[0,2]$ is

$$\int_0^2 f(x)\,dx \simeq f(0)+f(2)$$

while the Simpson's rule for $f(x)$ on $[0,2]$ is

$$\int_0^2 f(x)\,dx \approx \frac{1}{3}\left[f(0)+4f(1)+f(2)\right]$$

The results to 3-places for some funcs. are given in the following Table:

$f(x)$	x^2	x^4	$1/(x+1)$	$\sqrt{1+x^2}$	$\sin x$	e^x
Exact value	2.667	6.400	1.099	2.958	1.416	6.389
Trapezoidal	4.000	16.000	1.333	3.326	0.909	8.389
Simpson's	2.667	6.667	1.111	2.964	1.425	6.421

The standard derivation of quadrature error formulas is based on determining the class of polynomials for which these formulas produce exact results.

Def (4.1)

The deg. of accuracy, or precision, of a quadrature formula is the positive integer n such that:

$$E(P_k) = 0 \quad \forall P_k \qquad k \leq n$$

But $E(P_{n+1}) \neq 0$ for some polynomial of deg $(n+1)$.

Acc. to this def.:

Trapezoidal rule has deg. of precision one.
Simpson's " " " " " three.

Integration and summation are linear operations:

$$\int_a^b (\alpha f(x) + \beta g(x))\,dx = \alpha \int_a^b f(x)\,dx + \beta \int_a^b g(x)\,dx$$

$$\sum_{i=0}^{n} (\alpha f(x_i) + \beta g(x_i)) = \alpha \sum_{i=0}^{n} f(x_i) + \beta \sum_{i=0}^{n} g(x_i)$$

$\forall$ integrable $f(x)$ and $g(x)$ and real α, β.

This implies:

The deg. of Precision of a quadrature formula is n,

<u>if and only if</u> $E(x^k) = 0 \quad \forall\ k = 0, 1, \cdots n$

but $E(x^{n+1}) \neq 0$ (without proof)

Closed Newton-Cotes Formula ($n+1$ point):

This method uses nodes $x_i = x_0 + ih \quad i = 0, 1, \cdots n$

$$\begin{cases} x_0 = a \\ x_n = b \end{cases} \qquad h = \frac{b-a}{n}$$

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} a_i f(x_i)$$

$$a_i = \int_{x_0}^{x_n} L_i(x)\,dx = \int_{x_0}^{x_n} \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{(x - x_j)}{(x_i - x_j)}\,dx$$

Remark: The Trapezoidal and Simpson's rules are examples of a class of Newton-Cotes formula.

Theo. 4.2)

Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ denotes the $(n+1)$ point closed Newton-cotes formula with $x_0 = a$, $x_n = b$ and $h = \frac{b-a}{n}$.

There exists $\xi \in [a,b]$ for which;

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t^2(t-1)\cdots(t-n)dt$$

if $n =$ even and $f \in C^{n+2}[a,b]$

and

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1)\cdots(t-n)dt$$

if $n =$ odd and $f \in C^{n+1}[a,b]$

Note that;

i) When $n =$ even, the deg. of Precision $= n+1$
(Although the interpolation polynomial is of deg. <u>at most</u> $\underline{n}$)

ii) When $n =$ odd, the deg. of Precision $= n$

Some common closed Newton-Cotes formulas, with their error terms:

$n=1$ Trapezoidal rule

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}\left[f(x_0)+f(x_1)\right] - \frac{h^3}{12} f''(\xi) \qquad x_0 < \xi < x_1$$

Open Newton-Cotes Formula:

The nodes $x_i = x_0 + ih$ are used $i = 0, 1, \dots n$

$$h = \frac{b-a}{n+2}$$

$$x_0 = a + h \xrightarrow{\text{This impleis}} x_n = b - h$$

$$x_{-1} = a \quad , \quad x_{n+1} = b$$

$$\int_a^b f(x)dx = \int_{x_{-1}}^{x_{n+1}} f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i)$$

$$a_i = \int_a^b L_i(x)dx$$

Theo 4.3)

Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ denotes the $(n+1)$ point open Newton-Cotes formula with;

$$x_{-1} = a, \quad x_{n+1} = b \quad , \quad h = \frac{b-a}{n+2}$$

There exists $\xi \in (a,b)$ for which

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_{-1}^{n+1} t^2(t-1) \cdots (t-n)\,dt$$

If n = even and $f \in C^{n+2}[a,b]$

and

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_{-1}^{n+1} t(t-1)\cdots(t-n)\,dt$$

if n = odd and $f \in C^{n+1}[a,b]$

Some of the common open Newton-Cotes formulas with their error terms:

$n=0$ Midpoint rule

$$\int_{x_{-1}}^{x_1} f(x)\,dx = 2h f(x_0) + \frac{h^3}{3} f''(\xi) \qquad x_{-1} < \xi < x_1$$

$n=1$
$$\int_{x_{-1}}^{x_2} f(x)\,dx = \frac{3h}{2}\left[f(x_0) + f(x_1)\right] + \frac{3h^3}{4} f''(\xi) \quad x_{-1} < \xi < x_2$$

$n=2$
$$\int_{x_{-1}}^{x_3} f(x)\,dx = \frac{4h}{3}\left[2f(x_0) - f(x_1) + 2f(x_2)\right] + \frac{14h^5}{45} f^{(4)}(\xi)$$
$$x_{-1} < \xi < x_3$$

$n=3$
$$\int_{x_{-1}}^{x_4} f(x)\,dx = \frac{5h}{24}\left[11f(x_0) + f(x_1) + f(x_2) + 11f(x_3)\right] + \frac{95h^5}{144} f^{(4)}(\xi)$$
$$x_{-1} < \xi < x_4$$

$n=2$ Simpson's rule

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}\left[f(x_0)+4f(x_1)+f(x_2)\right] - \frac{h^5}{90} f^{(4)}(\xi) \qquad x_0<\xi<x_2$$

$n=3$ Simpson's three-eight rule

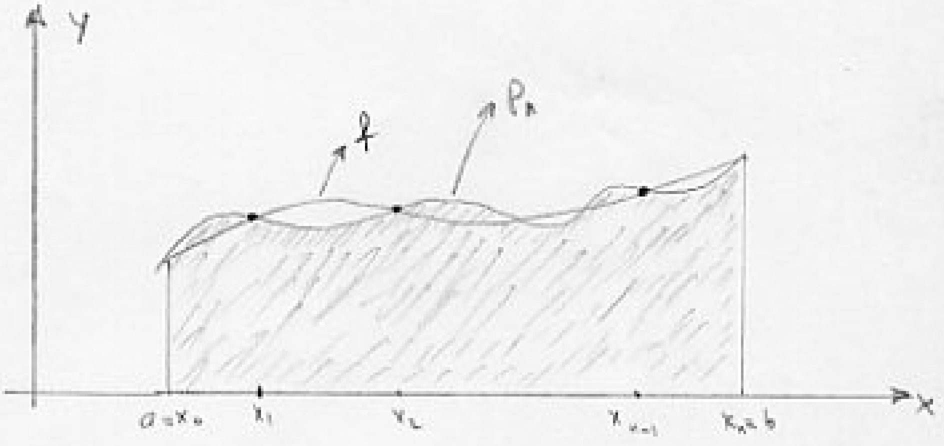
$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3h}{8}\left[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\right] - \frac{3h^5}{80} f^{(4)}(\xi)$$

$$x_0<\xi<x_3$$

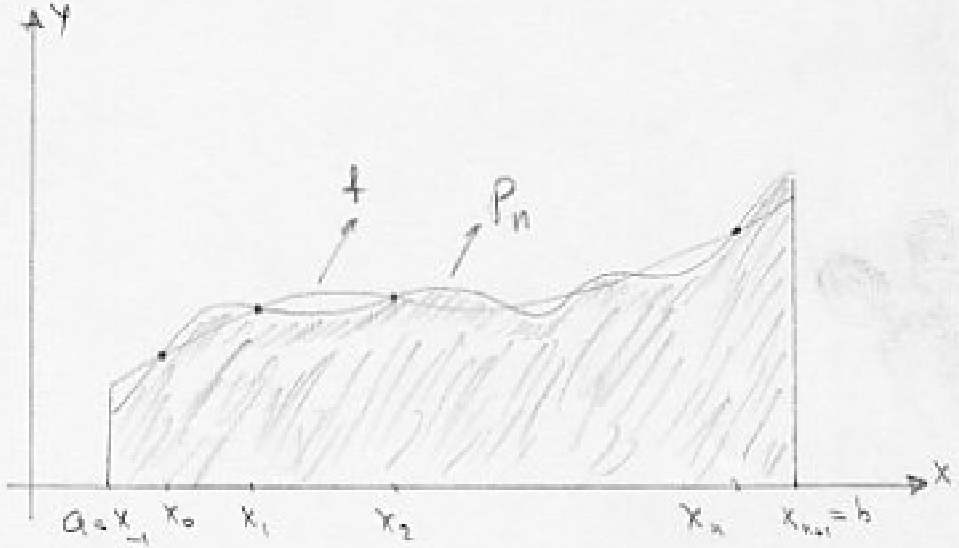
$n=4$

$$\int_{x_0}^{x_4} f(x)\,dx = \frac{2h}{45}\left[7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)\right] - \frac{8h^7}{945} f^{(6)}(\xi) \qquad x_0<\xi<x_4$$

Closed Newton-Cotes formula



Open Newton-Cotes formula



Ex.

Using the closed and open Newton-Cotes formulas to approximate $\int_0^{\pi/4} \sin x \, dx = 1 - \sqrt{2}/2$ gives the results:

n	0	1	2	3	4
Closed formulas		0.27768018	0.29293264	0.29291070	0.29289318
Error		0.01521303	0.00003942	0.00001748	0.00000004
Open formulas	0.30055887	0.29798754	0.29285866	0.29286923	
Error	0.00766565	0.00509432	0.00003456	0.00002399	

Generally closed formulas produce results superior to open formulas of the same order, (since they use more complete information about the func.)

The open formulas are primarily used for the numerical sol. of ordinary differential equs. -

4-4 Composite Numerical Integration

The Newton-Cotes formulas are generally unsuitable for use over a large integration intervals, (since high-deg. formulas would be required for use over such intervals and the values of the coeffs. in those formulas are difficult to obtain)

Also, the Newton-Cotes formulas use equally spaced nodes, a procedure that is inaccurate over large intervals, because of the oscillatory nature of high-deg. polynomials.

In this section we discuss a piecewise approach to numerical integration that uses the low-order Newton-Cotes formulas.

Ex. $\int_0^4 e^x dx = ?$

Simpson's rule, $h=2$

$$\int_0^4 e^x dx \approx \frac{2}{3}(e^0 + 4e^2 + e^4) = 56.76458$$

Since $\int_0^4 e^x dx = e^4 - e^0 = 53.59815$ exact

$\rightarrow$ error $= -3.17143$

Piecewise tequnique:

$$\int_0^4 e^x dx = \int_0^2 e^x dx + \int_2^4 e^x dx$$

$$\approx \frac{1}{3}\left[e^0 + 4e + e^2\right] + \frac{1}{3}\left[e^2 + e^3 + e^4\right] = 53.86385$$

error $= -0.26570$

Also

$$\int_0^4 e^x dx = \int_0^1 e^x dx + \int_1^2 e^x dx + \int_2^3 e^x dx + \int_3^4 e^x dx = 53.61622$$

error $= -0.01807$

Generalization:

1) Subdivide the interval $[a,b]$ into $\underline{m}$ subintervals

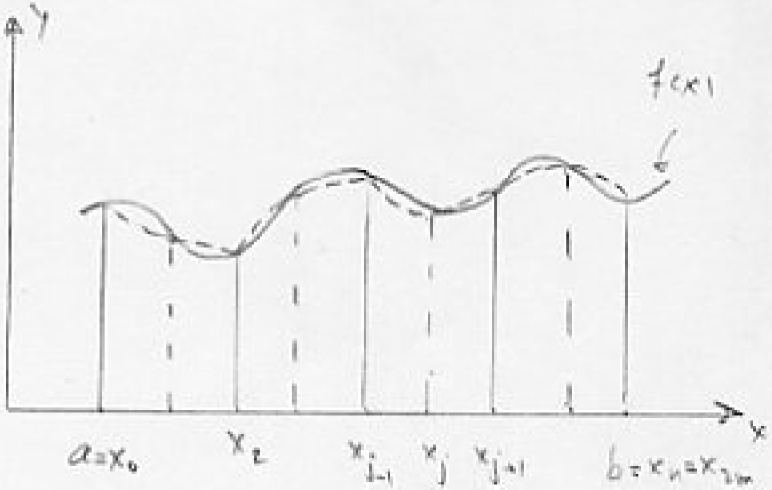
2) Use Simpsons rule on each consecutive pair of subintervals

Since Simpsons rule uses 3-points $\longrightarrow n = 2m$ m integer

$$h = \frac{b-a}{2m}$$

$$a = x_0 < x_1 \cdots < x_{2m} = b$$

$x_j = x_0 + jh \qquad j = 0, 1 \ldots 2m$



$$\int_a^b f(x)\,dx = \sum_{j=1}^{m} \int_{x_{2j-2}}^{x_{2j}} f(x)\,dx$$

$$= \sum_{j=1}^{m} \left\{ \frac{h}{3}\left[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})\right] - \frac{h^5}{90} f^{(4)}(\xi_j) \right\}$$

$x_{2j-2} < \xi_j < x_{2j}$ provided that $f \in C^4[a,b]$

For each $j = 1, 2, \dots m-1$: $f(x_{2j})$ appears $\begin{cases} 1\text{- in the term corresponding to the interval } [x_{2j-2}, x_{2j}] \\ 2\text{- in the term corresponding to the interval } [x_{2j}, x_{2j+2}] \end{cases}$

$$\longrightarrow \int_a^b f(x)\,dx = \frac{h}{3}\left[f(x_0) + 2\sum_{j=1}^{m-1} f(x_{2j}) + 4\sum_{j=1}^{m} f(x_{2j-1}) + f(x_{2m})\right] - \frac{h^5}{90}\sum_{j=1}^{m} f^{(4)}(\xi_j)$$

$x_{2j-2} < \xi_j < x_{2j}$ $\quad j = 1, \dots 2m$

$$E(f) = -\frac{h^5}{90}\sum_{j=1}^{m} f^{(4)}(\xi_j)$$

If $f \in C^4[a,b]$, by the Extreme Value Theo. (P54)

$$\min_{x\in[a,b]} f^{(4)}(x) \leq f^{(4)}(\xi_j) \leq \max_{x\in[a,b]} f^{(4)}(x)$$

$$m \min_{x\in[a,b]} f^{(4)}(x) \leq \sum_{j=1}^{m} f^{(4)}(\xi_j) \leq m \max_{x\in[a,b]} f^{(4)}(x)$$

$$\underset{x\in[a,b]}{\mathrm{Min}} f^{(4)}(x) \leq \frac{1}{m}\sum_{j=1}^{m} f^{(4)}(\xi_j) \leq \underset{x\in[a,b]}{\mathrm{Max}} f^{(4)}(x)$$

By the Intermediate Value Theo.$^{(855)}$, $\exists\ \mu \in (a,b)$

such that; $f^{(4)}(\mu) = \frac{1}{m}\sum_{j=1}^{m} f^{(4)}(\xi_j)$

$$\longrightarrow \quad E(f) = -\frac{h^5}{90}\, m f^{(4)}(\mu)$$

Since $h = \frac{b-a}{2m}$ $\Rightarrow E(f) = \frac{-h^4(b-a)}{180} f^{(4)}(\mu)$

These Observations produce the following result;

Theo. 4.4

If $f \in C^4[a,b]$, $\exists$ a $\mu \in (a,b)$ for which the Composite Simpson's rule for $n = 2m$, subintervals of $[a,b]$ can be expressed with error term as;

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(a) + 2\sum_{j=1}^{m-1} f(x_{2j}) + 4\sum_{j=1}^{m} f(x_{2j-1}) + f(b)\right] - \frac{(b-a)h^4}{180} f^{(4)}(\mu)$$

where

$a = x_0 < x_1 < \cdots < x_n = b$

$h = \frac{b-a}{n}$, $x_j = x_0 + jh$ $\quad j = 0, 1, \ldots n$

Composite Simpson's Algorithm 4.1

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

Input, a, b, $n = 2m$

Output approx. XI to I;

S1 $h = \frac{b-a}{n}$

S2 $XI0 = f(a) + f(b)$

$XI1 = 0$ $(\Sigma f(x_{2i-1}))$

$XI2 = 0$ $(\Sigma f(x_{2i}))$

S3 Do $i = 1, n-1$

S4 $X = a + ih$

S5 If i = even then $XI2 = XI2 + f(X)$

else $XI1 = XI1 + f(X)$

Continue

S6 $XI = h[XI0 + 2(XI2) + 4(XI1)]/3$

S7 Output XI

Stop

This is the most frequently used general-purpose quadrature algorithm.

Theo 4.5

Let $f \in C^2[a,b]$. With $h = \frac{b-a}{n}$, $x_j = a + jh$, $j = 0, 1, \dots n$, the composite Trapezoidal rule for n subinterval is

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a) + f(b) + 2\sum_{j=1}^{n-1} f(x_j)\right] - \frac{(b-a)h^2}{12} f''(\mu)$$

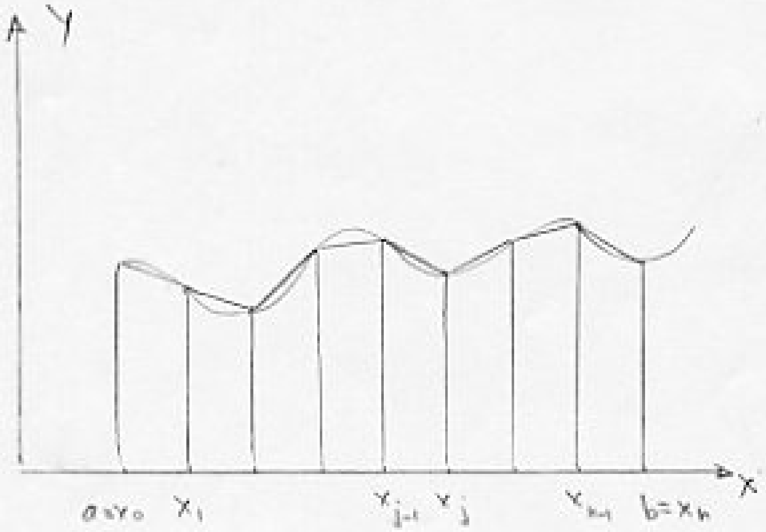
(no restriction on n) $\qquad \mu \in (a,b)$

Theo. 4.6

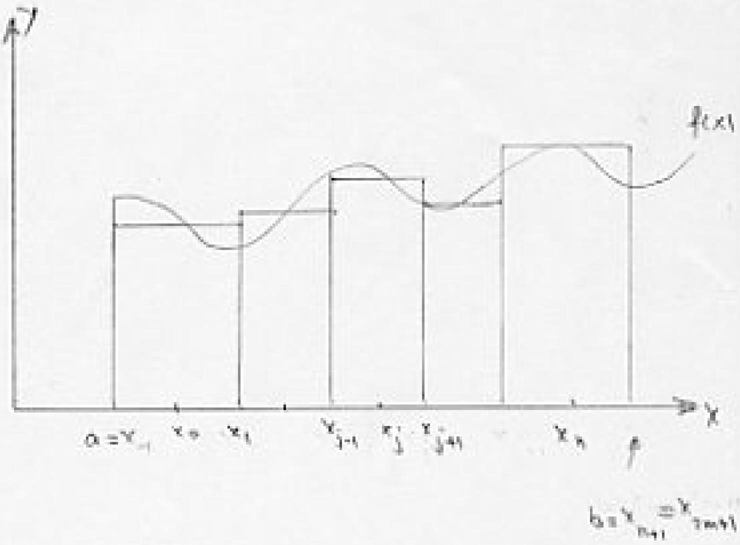
Let $f \in C^2[a,b]$. With $h = \frac{b-a}{2m+2}$ and $x_j = a + (j+1)h$, $j = 0, 1, \dots 2m+1$, the Composite Midpoit rule for $m+1$ subintervals is

$$\int_a^b f(x)\,dx = 2h\sum_{j=0}^{m} f(x_{2j}) + \frac{(b-a)h^2}{6} f''(\mu)$$

$\mu \in (a,b)$



Composite Trapezoidal rule



Composit Midpoint rule

Ex. $\int_0^{\pi} \sin x\,dx = ?$ Error $= 0.00002$ at most

using Simpson's rule.

$$\int_0^{\pi} \sin x\,dx = \frac{h}{3}\left[0 + 2\sum_{j=1}^{m-1} \sin x_{2j} + 4\sum_{j=1}^{m} \sin x_{2j-1} + 0\right] - \frac{\pi h^4}{180}\sin\mu$$

$$\left|\frac{\pi h^4}{180}\sin\mu\right| \leqslant \frac{\pi h^4}{180} = \frac{\pi^5}{2880 m^4} \leqslant 0.00002$$

$$\left(h = \frac{b-a}{2m} = \frac{\pi - 0}{2m}\right)$$

$\rightarrow m \geq 9 \qquad m = 10 \rightarrow n = 20 \quad \rightarrow h = \frac{\pi}{20}$

$$\int_0^{\pi} \sin x\,dx \approx \frac{\pi}{60}\left[2\sum_{j=1}^{9} \sin\left(\frac{j\pi}{10}\right) + 4\sum_{j=1}^{10} \sin\left(\frac{(2j-1)\pi}{20}\right)\right] = 2.000006$$

Using Trapezoidal rule;

$$\left|\frac{\pi h^2}{12}\sin\mu\right| \leqslant \frac{\pi h^2}{12} = \frac{\pi^3}{12 n^2} < 0.00002 \quad \rightarrow n \geqslant 360$$

For comparison; the Composite Trapezoidal rule; with $n = 20$ and $h = \frac{\pi}{20}$

$$\int_0^{\pi} \sin x\,dx \approx \frac{\pi}{40}\left[2\sum_{j=1}^{19} \sin\left(\frac{j\pi}{20}\right) + \sin 0 + \sin \pi\right]$$

$$= \frac{\pi}{40}\left[2\sum_{j=1}^{19} \sin\left(\frac{j\pi}{20}\right)\right] = 1.9958860$$

$$\int_0^{\pi} \sin x \, dx = 2 \quad \text{exact}$$

Stability with respect to round-off error:

Suppose we apply Composite Simpson's rule with $n=2m$;

$$\underset{\substack{\uparrow \\ \text{true} \\ \text{value}}}{f(x_i)} = \underset{\substack{\uparrow \\ \text{approx.} \\ \text{value}}}{\tilde{f}(x_i)} + \underset{\substack{\uparrow \\ \text{roundoff} \\ \text{error}}}{e_i} \qquad i = 0, 1, \ldots n$$

$$e(h) = \left| \frac{h}{3}\left[e_0 + 2\sum_{j=1}^{m-1} e_{2j} + 4\sum_{j=1}^{m} e_{2j-1} + e_{2m}\right]\right| \quad \text{accumulated error}$$

$$\leq \frac{h}{3}\left[|e_0| + 2\sum_{j=1}^{m-1}|e_{2j}| + 4\sum_{j=1}^{m}|e_{2j-1}| + |e_{2m}|\right]$$

If $e_i \leq \epsilon$

$$e(h) \leq \frac{h}{3}\left[\epsilon + 2(m-1)\epsilon + 4(m)\epsilon + \epsilon\right] = \frac{h}{3} 6 m\epsilon = 2mh\epsilon$$

But $2mh = b-a \rightarrow e(h) \leq (b-a)\epsilon$ (see P164)

$\rightarrow e$ = indep of h

$\rightarrow$ The procedure is stable as $h \rightarrow 0$

Remark: Truncation error $\sim h^4$

This is true for all the Composite Newton-Cotes integration tequniques.

(This was not true in numerical differentiation).

4-5 Adaptive Quadrature Methods:

In composite formulas we used equally spaced nodes.

If $f(x)$ contains both regions with $\begin{cases} \text{large functional variations} \\ \text{small functional variations} \end{cases}$

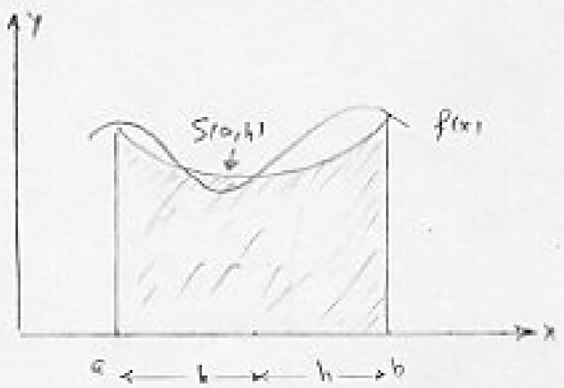
this is inappropriate.

For uniform distributed approx. error $\longrightarrow$ $\begin{cases} \text{a smaller step size for the large variation} \\ \text{regions than for with less variation} \\ \text{is needed} \end{cases}$

Adaptive Quadrature Methods, distinguish the amount of functional variation and adapt the step size to the varying requirements of the problem.

We discuss the method based on Composite Simpson's rule, but the technique can be easily modified to the other composite procedures.

$$\int_a^b f(x)\,dx = ? \qquad \text{within the tolerance } \epsilon > 0$$



Acc. to Simpson's rule;

$h = \dfrac{(b-a)}{2}$

$$\int_a^b f(x)\,dx = S(a,b) - \frac{h^5}{90} f^{(4)}(\mu) \qquad \mu \text{ in } (a,b) \tag{1}$$

where $S(a,b) = \frac{h}{3}\left[f(a) + 4f(a+h) + f(b) \right]$

Next step: Estimate the accuracy without determining $f^{(4)}(\mu)$

Apply Composite Simpson's rule with $m=2$, $\frac{b-a}{4} = \frac{h}{2}$ (step size)

$$\int_a^b f(x)\,dx = \frac{h}{6}\left[f(a) + 4f\left(a+\frac{h}{2}\right) + 2f(a+h) + 4f\left(a+\frac{3h}{2}\right) + f(b) \right] - \left(\frac{h}{2}\right)^4 \frac{(b-a)}{180} f^{(4)}(\tilde{\mu}) \qquad \tilde{\mu} \text{ in } (a,b)$$

To simplify notation, let

$$S\left(a, \frac{a+b}{2}\right) = \frac{h}{6}\left[f(a) + 4f\left(a+\frac{h}{2}\right) + f(a+h) \right]$$

$$S\left(\frac{a+b}{2}, b\right) = \frac{h}{6}\left[f(a+h) + 4f\left(a+\frac{3h}{2}\right) + f(b) \right]$$

$$\rightarrow \int_a^b f(x)\,dx = S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\tilde{\mu}) \tag{2}$$

The <u>error estimation</u> is derived by <u>assuming</u> that $\mu \approx \tilde{\mu}$

or, more precisely, that $f^{(4)}(\mu) \approx f^{(4)}(\tilde{\mu})$.

The success of the technique depends on the accuracy of this assumption.

If it is accurate;

$$(1)(2) \rightarrow S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\mu) \simeq S(a,b) - \frac{h^5}{90} f^{(4)}(\mu)$$

$$\rightarrow \frac{h^5}{90} f^{(4)}(\mu) \simeq \frac{16}{15}\left[S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right]$$

Using this in (2);

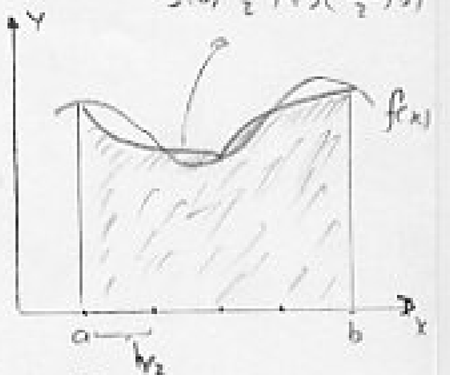
$$\left| \int_a^b f(x)\,dx - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| \simeq \frac{1}{15}\left| S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right|$$

Thus if; $\left| S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| < 15\epsilon$ (3)

$$\rightarrow \left| \int_a^b f(x)\,dx - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| < \epsilon \qquad (4)$$

In this case; $\int_a^b f(x)\,dx \simeq S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right)$

sufficiently accurate approx.



Ex. $\int_0^{\pi/2} \sin x\,dx = 1$

$$S\left(0, \frac{\pi}{2}\right) = \frac{\pi/4}{3}\left[\sin 0 + 4\sin\frac{\pi}{4} + \sin\frac{\pi}{2}\right] = \frac{\pi}{12}(2\sqrt{2}+1) = 1.002279878$$

$$S\left(0, \frac{\pi}{4}\right) + S\left(\frac{\pi}{4}, \frac{\pi}{2}\right) = \frac{\pi/8}{3}\left[\sin 0 + 4\sin\frac{\pi}{8} + 2\sin\frac{\pi}{4} + 4\sin\frac{3\pi}{8} + \sin\frac{\pi}{2}\right]$$

$= 1.0001345845$

So, $\frac{1}{15}\left| S\left(0, \frac{\pi}{2}\right) - S\left(0, \frac{\pi}{4}\right) - S\left(\frac{\pi}{4}, \frac{\pi}{2}\right)\right| = 0.000143020$

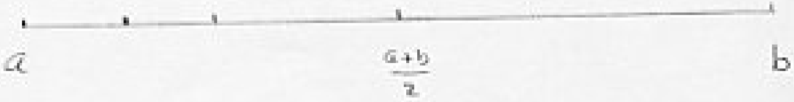
(a)

$$\left| \int_0^{\pi/2} \sin x\,dx - 1.0001354585 \right| = 0.0001354585 \quad \text{actual error}$$

(b)

(a) and (b) are very close, even though $D_x^4 \sin x = \sin x$ varies significantly in the interval $[0, \frac{\pi}{2}]$

Procedure:



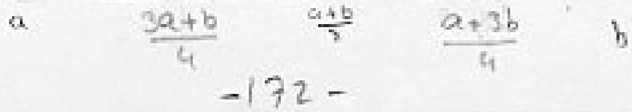
1) Error estimation is found for the interval $[a, b]$, if the inequality (3) holds $\longrightarrow$ $\int_a^b f(x)\,dx = S(a, \frac{a+b}{2}) + S(\frac{a+b}{2}, b) \pm \varepsilon$

2) When the inequality (3) doesn't hold, error estimation procedure is applied individually to the subintervals $[a, \frac{a+b}{2}]$ and $[\frac{a+b}{2}, b]$, and check a similar inequality like equ. (3) for each interval but for the error $\frac{\varepsilon}{2}$.

3) If the approx. for each interval is within the tolerance $\frac{\varepsilon}{2}$, then

$$\int_a^b f(x)\,dx = \int_a^{\frac{a+b}{2}} f(x)\,dx + \int_{\frac{a+b}{2}}^{b} f(x)\,dx$$

$$\int_a^b f(x)\,dx = S(a, \tfrac{3a+b}{4}) + S(\tfrac{3a+b}{4}, \tfrac{a+b}{2}) + S(\tfrac{a+b}{2}, \tfrac{a+3b}{4}) + S(\tfrac{a+3b}{4}, b)$$

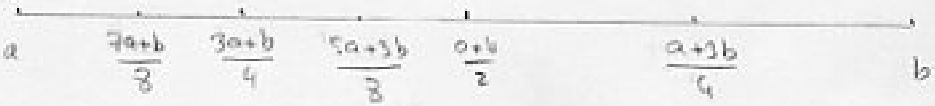


$\pm (\frac{\varepsilon}{2} + \frac{\varepsilon}{2})$

4) If <u>for example</u> the left interval approx. is not within the tolerance $\frac{\epsilon}{2}$, but the right interval is within the tolerance $\frac{\epsilon}{2}$, then, divide the left interval by <u>2</u> and check the <u>relevant</u> inequality like equ. (3) but for $\frac{\epsilon}{4}$. If the result is within the tolerance $\frac{\epsilon}{4}$ for both <u>second</u> subdivisions, then;

$$\int_a^b f(x)\,dx = \underbrace{\int_a^{\frac{3a+b}{4}} f(x)\,dx + \int_{\frac{3a+b}{4}}^{\frac{a+b}{2}} f(x)\,dx} + \underbrace{\int_{\frac{a+b}{2}}^{b} f(x)\,dx}$$

$$\int_a^b f(x)\,dx = \overbrace{\underbrace{S\left(a, \tfrac{7a+b}{8}\right) + S\left(\tfrac{7a+b}{8}, \tfrac{3a+b}{4}\right)} + \underbrace{S\left(\tfrac{3a+b}{4}, \tfrac{5a+3b}{8}\right) + S\left(\tfrac{5a+3b}{8}, \tfrac{a+b}{2}\right)}}$$
$$+ \underbrace{S\left(\tfrac{a+b}{2}, \tfrac{a+3b}{4}\right) + S\left(\tfrac{a+3b}{4}, b\right)} \pm \left(\frac{\epsilon}{2} + \frac{\epsilon}{4} + \frac{\epsilon}{4}\right)$$



5) In each step if the relevant inequality does not satisfy we divide the subinterval and get two new subintervals and reduce the <u>error</u> by a factor of $\frac{1}{2}$.

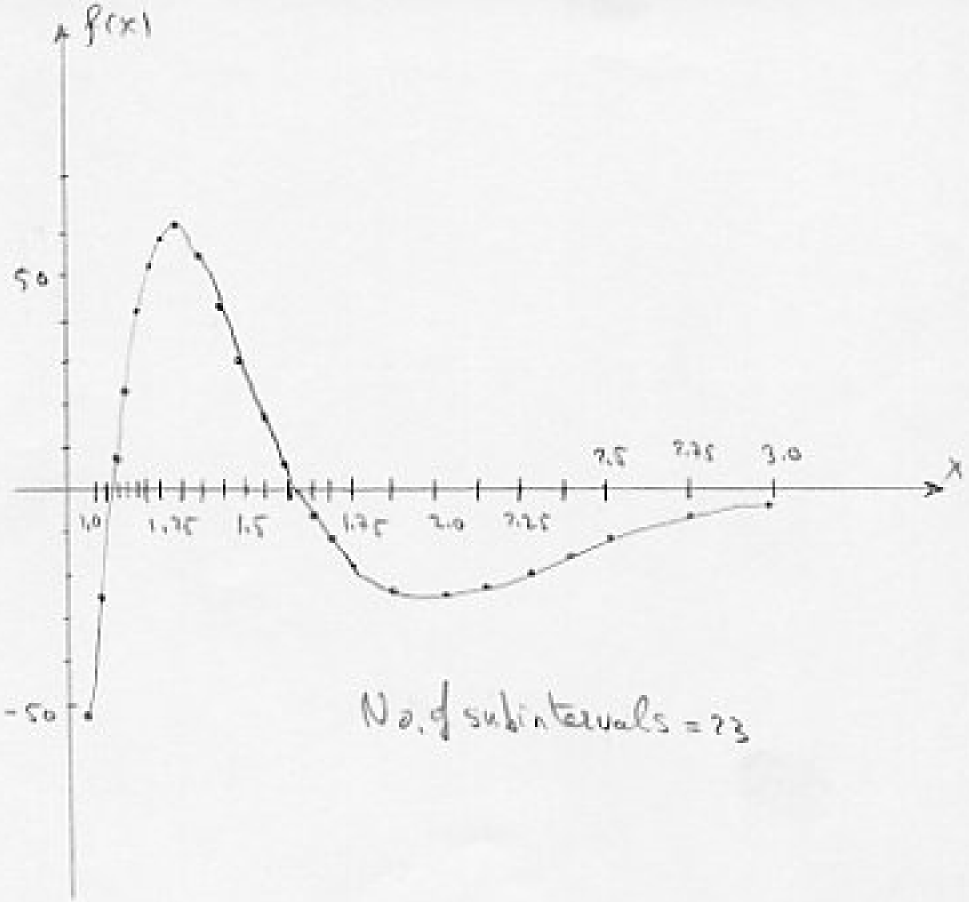
Although problem can be constructed for which the given tolerance will <u>never be met</u>, this technique is successful for most problems, because each subdivision increases the accuracy of the approx. by a factor of <u>15</u> while requiring an increased accuracy factor of only <u>2</u>.

Ex.

$$f(x) = \frac{100}{x^2} \sin\left(\frac{10}{x}\right)$$

$[1, 3]$

$$\int_1^3 f(x)\,dx = ? \qquad \epsilon = 10^{-4}$$



$$\int_1^3 f(x)\,dx = -1.426014$$

The result is accurate within 1.4×10^{-5}

For comparison:

Composite Simpson's rule with $h = \frac{1}{64} \longrightarrow \int_1^3 f(x)\,dx = -1.426059$

which differs from actual value by 2.4×10^{-5}.

4.2 Richardson's Extrapolation

This technique is employed to generate results of <u>high</u> accuracy by using low-order formulas.

Suppose: $N(h)$: a formula that produces approxs., of order $O(h^2)$ to M.

$$M = N(h) + k_1 h^2 + O(h^4) \qquad k_1 \neq k_1(h)$$

error $\qquad$ (1)

Replace $h \longrightarrow \frac{h}{2}$

$$M = N\left(\frac{h}{2}\right) + k_1 \frac{h^2}{4} + O\left(\left(\frac{h}{2}\right)^4\right) \qquad \text{more accurate}$$

$$M = N\left(\frac{h}{2}\right) + k_1 \frac{h^2}{4} + O(h^4) \qquad \text{(can be shown)}$$

(2)

(1)(2) $\rightarrow$ $$M = \frac{4N\left(\frac{h}{2}\right) - N(h)}{3} + O(h^4)$$

higher order

Define $N_1(h) = N(h)$

and $$N_2(h) = \frac{4N_1\left(\frac{h}{2}\right) - N_1(h)}{3}$$

$O(h^2)$	$O(h^4)$
$N_1(h)$	
$N_1\left(\frac{h}{2}\right)$	$N_2(h)$
$N_1\left(\frac{h}{4}\right)$	$N_2\left(\frac{h}{2}\right)$
$N_1\left(\frac{h}{8}\right)$	$N_2\left(\frac{h}{4}\right)$
$\vdots$	$\vdots$

If, in addition, a number k_2, indep. of h, exists so that,

$$M = N(h) + k_1 h^2 + k_2 h^4 + O(h^6)$$

$$\rightarrow M = \frac{4N_1(\frac{h}{2}) - N_1(h)}{3} + \frac{4k_2(h/2)^2 - k_2 h^4}{3} + O(h^6)$$

$$\rightarrow \quad M = N_2(h) - \frac{1}{4} k_2 h^4 + O(h^6) \qquad (3)$$

$$h \rightarrow \frac{h}{2} \qquad M = N_2(\tfrac{h}{2}) - \frac{1}{64} k_2 h^4 + O(h^6) \qquad (4)$$

$$(3)(4) \quad \rightarrow \quad M = \frac{16 N_2(h/2) - N_2(h)}{15} + O(h^6)$$

Thus if we define; $N_3(h) = \dfrac{4^2 N_2(h/2) - N_2(h)}{4^2 - 1}$

So $N_3(h) = \dfrac{16 N_2(\frac{h}{2}) - N_2(h)}{15}$

The procedure can be extended to <u>m such</u> columns, <u>provided</u> that the error form for the approx. of $N(h)$ to M can be expressed as;

$$M = N(h) + \sum_{j=1}^{m-1} k_j h^{2j} + O(h^{2m}) \qquad k_j \neq k_j(h)$$

The $O(h^{2j})$ approxs. are generated recursively by the formula

$$N_j(h) = \frac{4^{j-1} N_{j-1}(h/2) - N_{j-1}(h)}{4^{j-1} - 1} \qquad j = 2, 3, \dots m$$

4.6 Romberg Integration;

Romberg integration uses the Trapezoidal rule to give preliminary approx. and then applies the Richardson extrapolation process, to obtain improvements of the apporxs..

Trapezoidal rule using $\underline{m}$ subintervals;

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a)+f(b)+2\sum_{j=1}^{m-1} f(x_j)\right] - \frac{(b-a)}{12} h^2 f''(\mu)$$

$$a<\mu<b \quad , \; h = \frac{b-a}{m} \qquad x_j = a+jh \qquad j=0,1,\dots m$$

First step;

We obtain the Trapezoidal rule approx. with,

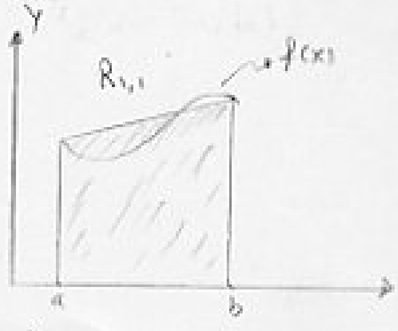
$$m_1 = 1, \quad m_2 = 2, \quad m_3 = 4 \;\dots\; m_n = 2^{n-1} \quad , \; n: \text{positive integer}$$

$$h_k = \frac{b-a}{m_k} = \frac{b-a}{2^{k-1}}$$

$$\int_a^b f(x)\,dx = \frac{h_k}{2}\left[f(a)+f(b)-2\left(\sum_{i=1}^{2^{k-1}-1} f(a+ih_k)\right)\right] - \frac{(b-a)}{12} h_k^2 f''(\mu_k)$$

μ_k in (a,b)

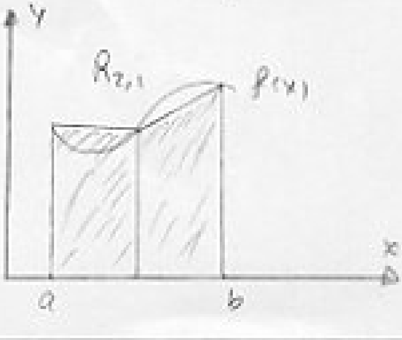
$$R_{1,1} = \frac{h_1}{2}\left[f(a)+f(b)\right] = \frac{(b-a)}{2}\left[f(a)+f(b)\right]$$



$$R_{2,1} = \frac{h_2}{2}\left[f(a)+f(b)+2f(a+h_2)\right]$$

$$= \frac{(b-a)}{4}\left[f(a)+f(b)+2f\left(a+\frac{(b-a)}{2}\right)\right]$$

$$= \frac{1}{2}\left[R_{1,1} + h_1 f(a+\tfrac{1}{2}h_1)\right]$$



$$R_{3,1} = \frac{h_3}{2}\left\{ f(a) + f(b) + 2\left[f\left(a + \frac{(b-a)}{4}\right) + f\left(a + \frac{(b-a)}{2}\right) + f\left(a + \frac{3(b-a)}{4}\right)\right]\right\}$$

$$= \frac{(b-a)}{8}\left\{ f(a) + f(b) + 2\left[f\left(a + \frac{(b-a)}{4}\right) + f\left(a + \frac{(b-a)}{2}\right) + f\left(a + \frac{3(b-a)}{4}\right)\right]\right\}$$

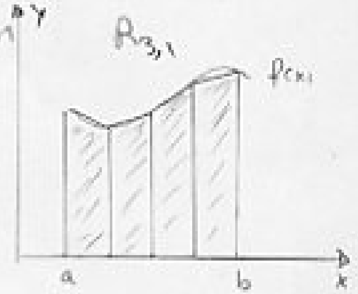
$$= \frac{1}{2}\left\{ R_{2,1} + h_2\left[f\left(a + \frac{h_2}{2}\right) + f\left(a + \frac{3h_2}{2}\right)\right]\right\}$$

and in general;

$$R_{k,1} = \frac{1}{2}\left[R_{k-1,1} + h_{k-1} \sum_{i=1}^{2^{k-2}} f\left(a + \left(i - \tfrac{1}{2}\right)h_{k-1}\right)\right]$$

$$k = 2, 3, \ldots n$$

<u>Ex.</u> Perform the first step of the Romberg integration for approximating $\int_0^{\pi} \sin x \, dx$ with $n = 6$;



$R_{1,1} = \frac{\pi}{2}\left[\sin 0 + \sin \pi\right] = 0$

$R_{2,1} = \frac{1}{2}\left[R_{1,1} + \pi \sin\frac{\pi}{2}\right] = 1.57079633$

$R_{3,1} = \frac{1}{2}\left[R_{2,1} + \frac{\pi}{2}\left(\sin\frac{\pi}{4} + \sin\frac{3\pi}{4}\right)\right] = 1.89611890$

$R_{4,1} = \frac{1}{2}\left[R_{3,1} + \frac{\pi}{4}\left(\sin\frac{\pi}{8} + \sin\frac{3\pi}{8} + \sin\frac{5\pi}{8} + \sin\frac{7\pi}{8}\right)\right] = 1.97423160$

$R_{5,1} = 1.99357034$

$R_{6,1} = 1.99839336$

$\int_0^{\pi} \sin x \, dx = 2$ exact

$\rightarrow$ The convergence is <u>slow</u>

The Second step;

To speed the convergence, the Richardson extrapolation procedure will now be performed.

It can be shown, if $f \in C^4[a,b] \xrightarrow{\text{then}}$ the composite Trapezoidal rule can be written with an alternate error term in the form;

$$\int_a^b f(x)\,dx = \underbrace{\frac{h_k}{2}\left[f(a)+f(b)+2\left(\sum_{i=1}^{2^{k-1}-1} f(a+ih_k)\right)\right]}_{R_{k,1}} - \frac{h_k^2}{12}\left[f'(b)-f'(a)\right] + \frac{(b-a)h_k^4}{720} f^{(4)}(\mu_k) \qquad (1)$$

$k=1,2,\ldots n. \qquad a<\mu_k<b$

Now we can eliminate the term involving h_k^2 by combining the eqns,

$$\int_a^b f(x)\,dx = R_{k-1,1} - \frac{h_{k-1}^2}{12}\left[f'(b)-f'(a)\right] + \frac{(b-a)h_{k-1}^4}{720} f^{(4)}(\mu_{k-1})$$

and

$$\int_a^b f(x)\,dx = R_{k,1} - \frac{h_k^2}{12}\left[f'(b)-f'(a)\right] + \frac{(b-a)h_k^4}{720} f^{(4)}(\mu_k)$$

$$= R_{k,1} - \frac{h_{k-1}^2}{48}\left[f'(b)-f'(a)\right] + \frac{(b-a)h_k^4}{720} f^{(4)}(\mu_k)$$

$\left(h_k = \frac{b-a}{2^{k-1}} \longrightarrow h_k = \frac{h_{k-1}}{2}\right)$

to obtain;

$$\int_a^b f(x)\,dx = \frac{4R_{k,1}-R_{k-1,1}}{3} + \frac{(b-a)}{2160}\left[4h_k^4 f^{(4)}(\mu_k) - h_{k-1}^4 f^{(4)}(\mu_{k-1})\right]$$

$$= \frac{4R_{k,1}-R_{k-1,1}}{3} + O(h_k^4)$$

To continue the Romberg scheme, we define

$$R_{k,2} = \frac{4R_{k,1} - R_{k-1,1}}{3} \qquad k = 2, 3 \ldots n$$

Now we apply the Richardson extrapolation procedure to these values.

If $f \in C^{2n+2}[a,b]$, then, for each $k = 1, 2, \ldots n$

the rule (1) can be generalized.

So the composite Trapezoidal rule on k subintervals can be expressed with an error term similar to that in (1)

$$\int_a^b f(x)\,dx = \frac{h_k}{2}\left[f(a) + f(b) + 2\left(\sum_{i=1}^{2^{k-1}-1} f(a + ih_k)\right)\right] + \sum_{i=1}^{k} K_i h_k^{2i} + O(h_k^{2k+2})$$

where $K_i \neq K_i(h_k)$ (without proof)

$$K_i = K_i(f^{(2i-1)}(a), f^{(2i-1)}(b))$$

In this case Romberg scheme can be continued to generate;

$$R_{i,j} = \frac{4^{j-1} R_{i,j-1} - R_{i-1,j-1}}{4^{j-1} - 1}$$

$i = 2, 3, \ldots n \qquad j = 2, \ldots i$

Truncation error associated with $R_{i,j}$ $= O(h_i^{2j})$ and involves an evaluation of $f^{(2i+2)}$

$$
\begin{array}{llllll}
R_{1,1} & & & & & \\
R_{2,1} & R_{2,2} & & & & \\
R_{3,1} & R_{3,2} & R_{3,3} & & & \\
R_{4,1} & R_{4,2} & R_{4,3} & R_{4,4} & & \\
\vdots & \vdots & \vdots & \vdots & & \\
R_{n,1} & R_{n,2} & R_{n,3} & R_{n,4} & \cdots & R_{n,n}
\end{array}
$$

The sequence $\{R_{n,n}\}_{n=1}^{\infty}$ converges much more rapidly than $\{R_{n,1}\}_{n=1}^{\infty}$.

Stopping Criterion;

$$
\text{both} \begin{cases} |R_{n-1,n-1} - R_{n,n}| < \epsilon \\ |R_{n-2,n-2} - R_{n-1,n-1}| < \epsilon \end{cases}
$$

To guard against the possibility that two consecutive row elements agree with each other but not with the value of the integral being approximated we check both of the mention Criterions.

4.7 Gaussian Quadrature;

Gaussian quadrature is concerned with choosing the points for evaluation (x_i), in an optimal manner (to increase the accuracy of approx.).

It presents a procedure for choosing $x_1, x_2 \cdots x_n$ in $[a,b]$ and consts. $c_1, c_2, \cdots c_n$ that are expected to minimize the error obtained in performing the approx.,

$$\int_a^b f(x)\,dx \simeq \sum_{i=1}^{n} c_i\, f(x_i) \qquad (1)$$

c_i : arbitrary
x_i : $f(x)$ must be defined at these points

Also, a polynomial of degree at most $(2n-1)$ contains $2n$ parameters (coeffs.).
This is the largest class of polynomials for which it is reasonable to expect equ (1) to be exact.
In fact $\longrightarrow$ For the proper choice of x_i and c_i, exactness on this set can be obtained.
This implies $\longrightarrow$ equ (1) can be designed to have deg of precision $(2n-1)$.

Orthogonal Functions:

The set of functions $\{\varphi_0, \varphi_1, - \varphi_n\}$ is said to be orthogonal on $[a,b]$ with respect to the continuous <u>weight func.</u> $W(x) \geq 0$ ($w(x) \not\equiv 0$), provided

$$\int_a^b \varphi_k(x)\,\varphi_j(x)\,w(x)\,dx = \begin{cases} 0 & \text{for } j \neq k \\ >0 & \text{"} \quad j = k \end{cases}$$

It can be shown that;

If $\{\varphi_0, \varphi_1, .. \varphi_n\}$ is an orthogonal set of polynomials defined on $[a,b]$ and φ_i is of degree $\underline{i}$ $(i = 0, 1 .. n)$;

Then $\Rightarrow$ $\forall\, Q$ (polynomial of deg. at most n) $\exists\ \alpha_0, \alpha_1 -- \alpha_n$ (unique consts.)

with $Q(x) = \sum_{i=0}^{n} \alpha_i \varphi_i(x)$.

(this is used in the proof of the following Theo.)

Theo 4.7

If $\{\varphi_0, \varphi_1 \cdots \varphi_n\}$ is a set of orthogonal polynomials defined on $[a,b]$ with respect to the continuous func. $W(x)$, and φ_k is a polynomial of deg. k $(k = 0, 1 \dots n)$,

then $\Rightarrow$ φ_k has <u>k distinct</u> zeros, when $k \geq 1$, and these zeros lie in the interval (a,b).

Legendre Polynomials:

Orthogonal polynomials defined on $[-1,1]$

$w(x) \equiv 1$

$P_0(x) = 1$, $P_1(x) = x$ $\quad P_k(x) = (x - B_k) P_{k-1}(x) - C_k P_{k-2}(x)$

$k = 2, 3, \ldots$

$$B_k = \frac{\int_{-1}^{1} x \left[P_{k-1}(x) \right]^2 dx}{\int_{-1}^{1} \left[P_{k-1}(x) \right]^2 dx} \qquad C_k = \frac{\int_{-1}^{1} x P_{k-1}(x) P_{k-2}(x) dx}{\int_{-1}^{1} \left[P_{k-2}(x) \right]^2 dx}$$

Theo. 4.8

If P is any polynomial of deg. $\leq 2n-1$, then

$$\int_{-1}^{1} P(x) dx = \sum_{i=1}^{n} c_i P(x_i) \qquad (1)$$

where

$$c_i = \int_{-1}^{1} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{(x - x_j)}{(x_i - x_j)} dx \qquad (2)$$

and $\cancel{x_0}, x_1 \text{ --- } x_n$ are the zeros of the nth Legendre polynomial.

Quadrature Rule;

The consts. c_i needed for the quadrature rule can be generated from equ.(2), but both c_i and x_i (roots) of the Legendre polynomials are extensively tabulated.

Since the simple linear tr. $t = \frac{1}{b-a}(2x-a-b)$ will translate

any $[a,b] \xrightarrow{\text{to}} [-1,1]$

the Legendre polynomials can be used to approximate

$$\int_a^b f(x)\,dx = \int_{-1}^{1} f\left(\frac{(b-a)t+b+a}{2}\right)\frac{b-a}{2}\,dt$$

for any func. that can be evaluated at the required points.

n	Roots	Coeffs.
2	0.5773502692	1.000,000,000,0
	-0.5773502692	"
3	0.7745966692	0.5555555556
	0.000,000,000,0	0.888,888,888,9
	-0.7745966692	0.555,555,555,6
4	....	----

Ex. $\int_1^{1.5} e^{-x^2}\,dx = ?$

$$\int_1^{1.5} e^{-x^2}\,dx = \frac{1}{4}\int_{-1}^{1} e^{(-(t+5)^2/16)}\,dt$$

$$n=2 \rightarrow \int_{-1}^{1} \simeq \frac{1}{4}\left[e^{-(5+0.5773502692)^2/16} + e^{-(5-0.5773502692)^2}\right] = 0.1094003$$

$$n=3 \quad \int_{-1}^{1} \simeq \frac{1}{4}\left[(0.555,555,5556)e^{-(5+0.7745966692)^2/16} + (0.888,888,8889)e^{-(5)^2/16} + (0.555,555,555,6)e^{-(5-0.7745966692)^2/16}\right]$$

$$= 0.1093642 \qquad \left(\int_1^{1.5} = 0.1093643 \text{ exact value}\right)$$

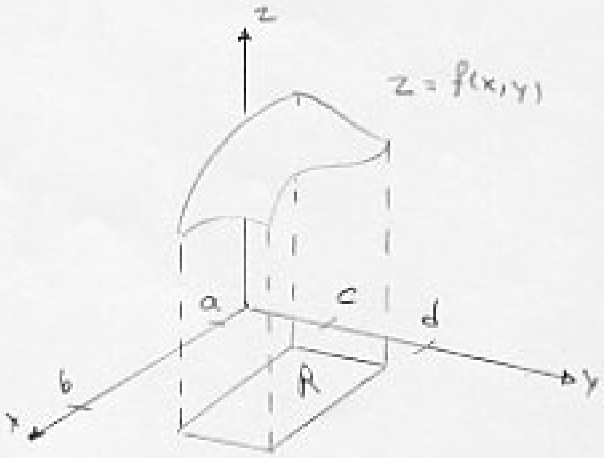
4.8 Multiple Integrals:

Double Integrals:

Consider $\iint_R f(x,y)\,dA$ $\quad R = \{(x,y) \mid a \le x < b,\ c \le y \le d\}$

(R; rectangular region in the plane)

To illustrate the approx. technique, we employ Composite Simpson's rule, (although any other composite Newton-Cotes formula could be used in its place).



Suppose that integers n and m are chosen to determine;

$h = \frac{b-a}{2n}$, $k = \frac{d-c}{2m}$

$$\iint_R f(x,y)\,dA = \int_a^b \left(\int_c^d f(x,y)\,dy \right) dx$$

First;

We use the Composite Simpson's rule to evaluate;

$$\int_c^d f(x,y)\,dy$$

treating x as a const. .

let, $Y_i = c + jk$, $j = 0, 1, \ldots 2m$

$$\int_c^d f(x,y)\,dy = \frac{k}{3}\left[f(x,y_0) + 2\sum_{j=1}^{m-1} f(x,y_{2j}) + 4\sum_{j=1}^{m} f(x,y_{2j-1}) + f(x,y_{2m})\right] - \frac{(d-c)k^4}{180}\frac{\partial^4 f(x,\mu)}{\partial y^4}$$

μ in (c,d)

$$\int_a^b\int_c^d f(x,y)\,dy\,dx = \frac{k}{3}\int_a^b f(x,y_0)\,dy + \frac{2k}{3}\sum_{j=1}^{m-1}\int_a^b f(x,y_{2j})\,dx + \frac{4k}{3}\sum_{j=1}^{m}\int_a^b f(x,y_{2j-1})\,dx + \frac{k}{3}\int_a^b f(x,y_{2m})\,dx - \frac{(d-c)k^4}{180}\int_a^b \frac{\partial^4 f(x,\mu)}{\partial y^4}\,dx$$

The Composite Simpson's rule is now employed on each integral in this eqn.

let $x_i = a + ih$, $i = 0, 1, \ldots 2n$

Then for each $j = 0, 1, \ldots 2m$; we have;

$$\int_a^b f(x,y_j)\,dx = \frac{h}{3}\left[f(x_0,y_j) + 2\sum_{i=1}^{n-1} f(x_{2i},y_j) + 4\sum_{i=1}^{n} f(x_{2i-1},y_j) + f(x_{2n},y_j)\right] - \frac{(b-a)h^4}{180}\frac{\partial^4 f}{\partial x^4}(\xi_j, y_j)$$

ξ_j in (a,b)

$$\int_a^b\int_c^d f(x,y)\,dy\,dx \approx \frac{hk}{9}\Big[f(x_0,y_0) + 2\sum_{i=1}^{n-1} f(x_{2i},y_0) + 4\sum_{i=1}^{n} f(x_{2i-1},y_0)$$

$$+ f(x_{2n},y_0) + 2\sum_{j=1}^{m-1} f(x_0,y_{2j}) + 4\sum_{j=1}^{m-1}\sum_{i=1}^{n-1} f(x_{2i},y_{2j})$$

$$+ 8\sum_{j=1}^{m-1}\sum_{i=1}^{n} f(x_{2i-1},y_{2j}) + 2\sum_{j=1}^{m-1} f(x_{2n},y_{2j})$$

$$+ 4\sum_{j=1}^{m} f(x_0,y_{2j-1}) + 8\sum_{j=1}^{m}\sum_{i=1}^{n-1} f(x_{2i},y_{2j-1})$$

$$+ 16\sum_{j=1}^{m}\sum_{i=1}^{n} f(x_{2i-1},y_{2j-1}) + 4\sum_{j=1}^{m} f(x_{2n},y_{2j-1})$$

$$+ f(x_0,y_{2m}) + 2\sum_{i=1}^{n-1} f(x_{2i},y_{2m}) + 4\sum_{i=1}^{n} f(x_{2i-1},y_{2m})$$

$$+ f(x_{2n},y_{2m}) \Big]$$

$$E = \frac{-k(b-a)h^4}{540}\Big[\frac{\partial^4 f(\xi_0,y_0)}{\partial x^4} + 2\sum_{j=1}^{m-1}\frac{\partial^4 f(\xi_{2j},y_{2j})}{\partial x^4}$$

$$+ 4\sum_{j=1}^{m}\frac{\partial^4 f(\xi_{2j-1},y_{2j-1})}{\partial x^4} + \frac{\partial^4 f(\xi_{2m},y_{2m})}{\partial x^4}\Big] - \frac{(d-c)k^4}{180}\int_a^b \frac{\partial^4 f(x,\mu)}{\partial y^4}\,dx$$

If $\dfrac{\partial^4 f}{\partial x^4}$ is continuous, using the Intermediate Value Theo.; (P55)

$$E = \frac{-k(b-a)h^4}{540}\Big[6m\frac{\partial^4 f}{\partial x^4}(\bar{\eta},\bar{\mu})\Big] - \frac{(d-c)k^4}{180}\int_a^b \frac{\partial^4 f(x,\mu)}{\partial y^4}\,dx$$

$(\bar{\eta},\bar{\mu})$ in R.

If $\frac{\partial^4 f}{\partial y^4}$ is also continuous, using the Weighted Mean Value Theo.; (P55)

$$\int_a^b \frac{\partial^4 f(x,\mu)}{\partial y^4}\,dx = (b-a)\frac{\partial^4 f}{\partial y^4}(\hat{\eta},\hat{\mu})$$

$(\hat{\eta},\hat{\mu})$ in R.

$$E = \frac{-k(b-a)h^4}{540}\left[6m\frac{\partial^4 f}{\partial x^4}(\bar{\eta},\bar{\mu})\right] - \frac{(d-c)(b-a)}{180}k^4\frac{\partial^4 f}{\partial y^4}(\hat{\eta},\hat{\mu})$$

$$= \frac{-(d-c)(b-a)}{180}\left[h^4\frac{\partial^4 f}{\partial x^4}(\bar{\eta},\bar{\mu}) + k^4\frac{\partial^4 f}{\partial y^4}(\hat{\eta},\hat{\mu})\right]$$

for $(\bar{\eta},\bar{\mu})$ and $(\hat{\eta},\hat{\mu})$ in R.

Double Integrals with Non-Rectangular Limits;

$$\int_a^b \int_{c(x)}^{d(x)} f(x,y)\,dx\,dy \qquad (1)$$

or
$$\int_c^d \int_{a(y)}^{b(y)} f(x,y)\,dx\,dy \qquad (2)$$

We consider the first one, and apply the <u>basic</u> Simpson's rule;
$$h = \frac{b-a}{2}, \quad k(x) = \frac{d(x)-c(x)}{2}$$

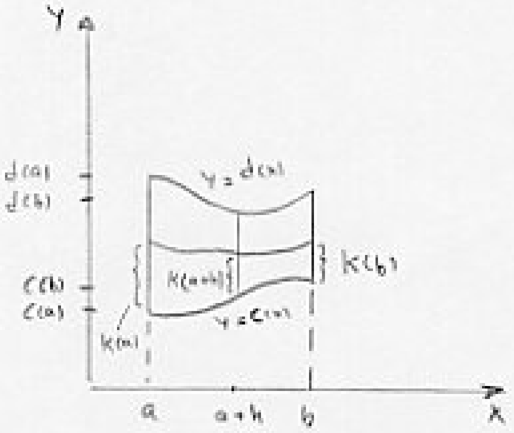
$$\int_a^b \int_{c(x)}^{d(x)} f(x,y)\,dx\,dy \approx \int_a^b \frac{k(x)}{3}\Big[f(x,c(x)) + 4f(x,c(x)+k(x)) + f(x,d(x))\Big]dx$$

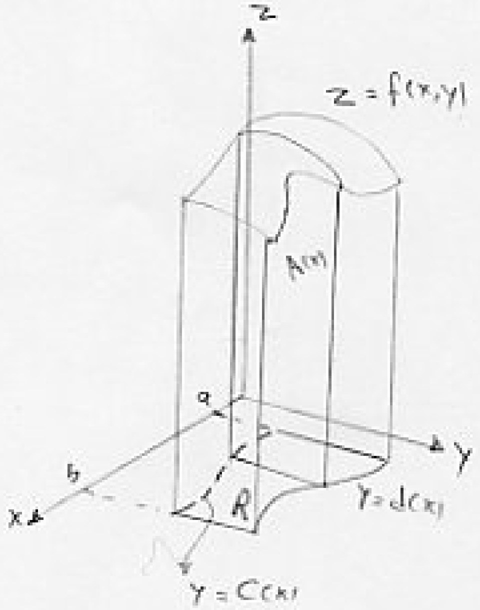
$$\approx \frac{h}{3}\Big\{ \frac{k(a)}{3}\Big[f(a,c(a)) + 4f(a,c(a)+k(a)) + f(a,d(a))\Big]$$

$$+ \frac{4k(a+h)}{3}\Big[f(a+h,c(a+h)) + 4f(a+h,c(a+h)+k(a+h))$$

$$+ f(a+h,d(a+h))\Big]$$

$$+ \frac{k(b)}{3}\Big[f(b,c(b)) + 4f(b,c(b)+k(b)) + f(b,d(b))\Big]\Big\}$$





The same techniques can be applied for the approx. of <u>triple</u> integrals, as well as <u>higher</u> integrals.