NUMERICAL DIFFERENTIATION AND NUMERICAL INTEGRATION

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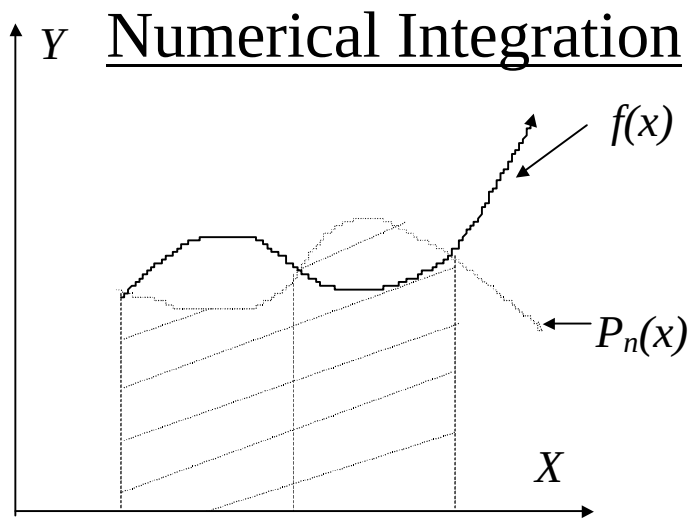
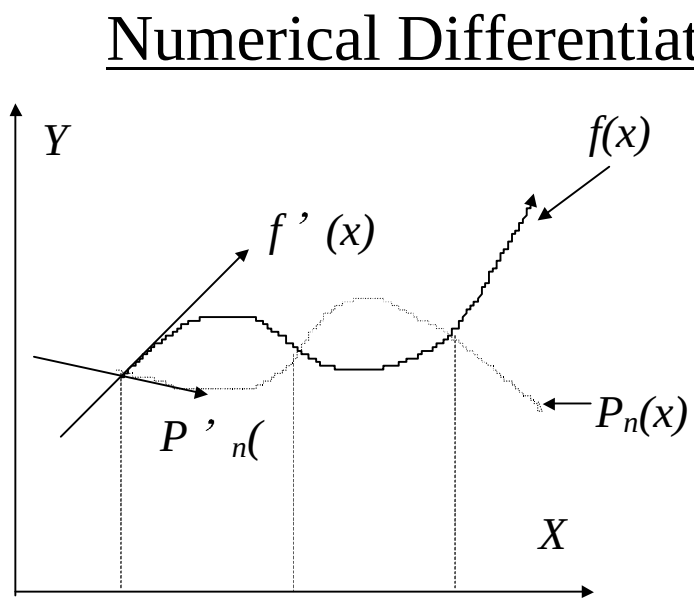
2.1 INTRODUCTION



. Find area under a series of tabulated points.



. Find the gradient at the discrete given points (x_i, y_i)
. In both cases analytical functions are not known, thus we rely completely on tabulated data points (x_i, y_i).

2.2 DERIVATIVES FROM INTERPOLATION

Consider the Newton-Gregory Forward Interpolation:

$$P_n(x) = f_o + sDf_o + \frac{s(s-1)}{2!} D^2 f_o + \ldots$$
$$+ \ Error$$

Error Term

$$e_n(x) = \binom{s}{n+1} h^{n+1} f^{n+1}(x)$$

$$where \ x_o < x < x_n$$

and $$s = \frac{x - x_o}{h}$$

On differentiating,

$$P_n^{'}(x) = \frac{d}{ds}[P_n(x)]\frac{ds}{dx} + \frac{d}{dx}[e_n(x)]$$

$$\frac{d}{ds}[P_n(x)]\frac{ds}{dx} = \frac{1}{h}\left\{\Delta f_o + \frac{1}{2}\left[(s-1)+s\right]\Delta^2 f_o\right.$$

$$\left. + \frac{1}{6}\left[(s-1)(s-2) + s(s-2) + s(s-1)\right]\Delta^3 f_o + \Lambda \right\}$$

For *one-sided forward difference*, at a specific point, $x = x_o$, $\therefore s = 0$.

$$P'_n(x_o) = \frac{1}{h}\left\{\Delta f_o - \frac{1}{2}\Delta^2 f_o + \frac{1}{3}\Delta^3 f - ..\right\} + \frac{d}{dx}[e_n(x)]$$

... (1)

The nth term in the bracket of Eq(1)

$$= \frac{(-1)^{n-1}\ \Delta^n f_o}{n}$$

Thus, Eq (1) gives the derivative of function at x_o using an nth degree polynomial passing through (x_o, f_o) and n additional points to the right. That is why it is known as *one-sided forward difference*.

EXAMPLE 1: DIFFERENCE TABLE

Obtain $f'(0)$ from the data below.
(The data are generated using $f(x) = e^x$).

x	f	Df	D^2f
0.0	1.000000		
		0.105172	
0.1	1.105172		0.011059
		0.116231	
0.2	1.221403		0.012225
		0.128456	
0.3	1.349859		

We know that the exact value

$$f'(0) = 1.00$$

Numerically, using 1 term only:

$$f'(0) = \frac{1}{0.1}\{Df_o\}$$

$$= \left(\frac{1\times 0.105172}{0.1}\right)$$

$$= 1.05172$$

Using 2 terms:

$$f'(0) = \frac{1\left(\Delta f_o - \frac{1}{2}\Delta^2 f_o\right)}{0.1}$$

$$= 1.05172 - \frac{1}{0.2}\,0.011059$$

$$= 0.99643$$

Using 3 terms, verify that $f'(0) = 1.00031$.

Error Term

Truncation error for

$$P_n'(x) = \frac{d}{dx}[e_n(x)]$$

$$= \frac{d}{dx}\left[\binom{s}{n+1} h^{n+1} f^{n+1}(x)\right]$$

$$= h^{n+1} f^{n+1}(x) \frac{d}{ds}\binom{s}{n+1}\frac{ds}{dx}$$

$$+ \binom{s}{n+1} h^{n+1} \frac{d}{dx}[f^{n+1}(x)]$$

The 2nd term cannot be determined because the way x varies with x is unknown.

But at $x = x_o$, $s = 0$ Þ $\binom{s}{n+1} = 0$, so the 2nd term vanishes.

1st term:

$$\frac{d}{ds}\binom{s}{n+1} = \binom{s}{n+1}\sum_{i=0}^{n}\frac{1}{(s-i)}$$

(Please prove it!)

At $s = 0$, $\quad \frac{d}{ds}\binom{s}{n+1} = \frac{(-1)^n}{n+1}$

Error of $P'_n(x)$

$$= h^n f^{n+1}(x)\frac{(-1)^n}{n+1}$$

where $x_o < x < x_n$

Colloraries:

- Although the interpolating formula is **exact** at x_o (by using the exact order) the derivative at x_o is subject to error.

- The term $f'(x) = D f_o/h$ in Eq.(1) is in terms of finite differences and can be used directly.

Generally, $f'(x_O)$ is expressed as:

$$f'(x_O) = \frac{1}{h}\left\{\Delta f_o - \frac{1}{2}\Delta^2 f_o + \frac{1}{3}\Delta^3 f_o + \Lambda + \frac{(-1)^{n-1}}{n}\Delta^n f_o\right\}$$

$$+ \frac{(-1)^n h^n}{(n+1)} f^{n+1}(x) \qquad x_o < x < x_n$$

1st term on R.H.S. gives an ***approximation*** for $f'(x_O)$.

2nd term on R.H.S. is the ***truncation*** error.

EXAMPLE 2: FORWARD DIFFERENCE DERIVATIES

Obtain the derivative of y at $x = 1.7$ and estimate the errors. (The equation is $y = e^x$).

x	y	Dy	D^2y	D^3y	D^4y
1.3	3.669				
		0.813			
1.5	4.482		0.179		
		0.992		0.041	
1.7	5.474		0.220		0.007
		1.212		0.048	
1.9	6.686		0.268		0.012
		1.480		0.060	
2.1	8.166		0.328		0.012
		1.808		0.072	
2.3	9.974		0.400		
		2.208			
2.5	12.182				

1 term

$$y'(1.7) = \frac{1}{h}\,\Delta\, f_o = \frac{1.212}{0.2} = 6.060$$

2 terms

$y'(1.7)$

$$= \frac{1}{h}\left(\Delta\, f_o - \frac{1}{2}\Delta^2 f_o\right) = \frac{1}{0.2}\left(1.212 - \frac{1}{2}\,0.268\right)$$

$$= 5.390$$

4 terms

verify that $y'(1.7) = 5.475$

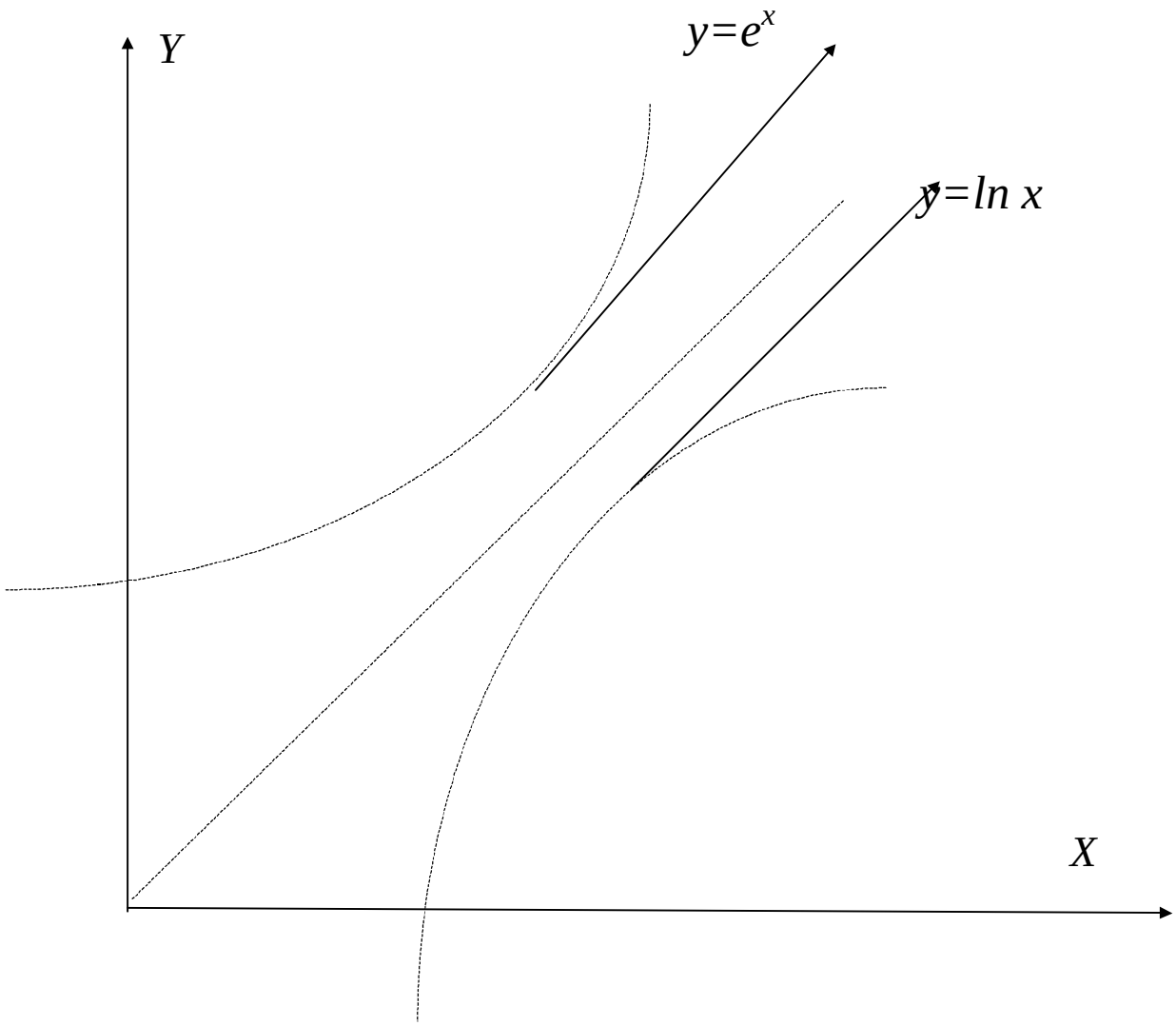
No. of terms	$f'(1.7)$	Error term	min. error	max. error	actual error
1	$\frac{(1\times 1.212)}{0.2}$ $= 6.06$	i	$\frac{-0.2\ e^{1.7}}{2}$ $= -0.547$	$\frac{-0.2\ e^{1.9}}{2}$ $= -0.669$	-0.586
2	$\frac{\left(1.212-\frac{0.268}{2}\right)}{0.2}$ $= 5.39$	ii	$\frac{0.04\ e^{1.7}}{3}$ $= 0.073$	$\frac{0.04\ e^{2.1}}{3}$ $= 0.109$	0.084
3	$5.39 + \frac{(0.06)}{3(0.2)}$ $= 5.49$	iii	$\frac{-0.008\ e^{1.7}}{4}$ $= -0.011$	$\frac{-0.008\ e^{2.3}}{4}$ $= -0.02$	-0.016

Eror terms

(i)– $\frac{1}{2}(0.2)^1\ f''(x)$ $\qquad 1.7 < x < 1.9$

(ii) $\frac{1}{3}(0.2)^2\ f'''(x)$ $\qquad 1.7 < x < 2.1$

(iii)– $\frac{1}{4}(0.2)^3\ f^{iv}(x)$ $\qquad 1.7 < x < 2.3$



For a one-sided forward difference $P_n'(x)$, it does not fit those points that are symmetrical about x_o.

Since the interpolation is more accurate near the centre of fit, we introduce central difference method.

2.3 CENTRAL DIFFERENCE

Consider

$$f'(xs) = \frac{1}{h}\left\{\Delta f_o + \frac{1}{2}(s-1+s)\Delta^2 f_o\right\} + \Lambda \quad error$$

The above formula is a 2nd degree polynomial which fits at x_o, x_1 and x_2.

Now if we fit x_s at x_1 using centre of fit theorem,

$$f'(x_1) = \frac{1}{h}\left\{\Delta f_o + \frac{\Delta^2 f_o}{2}\right\} + error$$

$$where\ s = \frac{(x_1 - x_o)}{h} = 1$$

$$f'(x_1) = \frac{1}{h}\left\{ f_1 - f_o + \frac{1}{2}\left(f_2 - 2f_1 + f_o \right) \right\}$$

$$= \frac{\left(f_2 - f_o \right)}{2h} + error$$

The *error* in the quadratic interpolation is

$$e_2(s) = \frac{s(s-1)(s-2)}{3!}\Delta^3 f_o$$

$$\frac{de_2(s)}{dx} = \frac{1}{h}.\frac{\Delta^3 f_0}{6}\left[s(s-1) + (s-1)(s-2) + s(s-2) \right]$$

Using centre of fit theorem, we fit x_s at x_1, i.e.

$$s = \frac{x_1 - x_o}{h} = 1$$

$$\frac{de_2(x_x)}{dx} = \frac{1}{h}.\frac{\Delta^3 f_0}{6}\left[1(-1) \right] = -\frac{1}{6}h^2 f'''(x)$$

$$\text{Note error} = -\frac{1}{6} h^2 f'''(x)$$

$$\text{where} \quad x_o \le \xi \le x_2$$

Contrast this with the forward difference error in $P_2'(x)$

i.e. = $\frac{1}{3} h^2 f'''(x)$

Corollaries:

- The coefficient in the central difference error term is *2 times* smaller than the corresponding error term in forward difference.

- Central difference formulas are superior to forward difference in calculating values for derivatives.

EXAMPLE 3: CENTRAL DIFFERENCE DERIVATIVE

Apply centre difference to find *y'(1.7)* for Eg.2.

$$f'(1.7) \approx \frac{(6.686 - 4.482)}{2(0.2)} = 5.510$$

Estimate error $-\frac{1}{6}\, 0.2^2\, e^{1.9} = -0.046$

(Upper limit)

$$-\frac{1}{6}\, 0.2^2\, e^{1.5} = -0.030$$

(Lower limit)

Actual error = $e^{1.7}$ - 5.510 = *-0.036*.

Central - difference formulae can only be derived using higher degree polynomials of *even order*. Why is it so ?

Corollaries:

- Observe error of interpolation is $0(h^{n+1})$ and the error of 1st derivative is $0(h^{n})$.

- Thus, if $h < 0.1$ which is normally the case then there will be greater errors for derivative in comparison with interpolation.

2.4 FORMULAE FOR HIGHER DERIVATIVES

$$f(x) = f_o + s\Delta f_o + \frac{s(s-1)}{2}\Delta^2 f_o + \frac{s(s-1)(s-2)}{6}\Delta^3 f_o + \ldots\ldots\ldots$$

$$f'(x) = \frac{df(x)}{dx} = \frac{df(x)}{ds}\frac{ds}{dx}$$

These can be obtained by repeated differentiation of an interpolation formula.

$$f'(x) = \frac{1}{h}\{Df_o + \frac{1}{2}[(s-1) + s]D^2 f_o$$

$$+ \frac{1}{6}[(s-1)(s-2) + s(s-2)$$

$$+ s(s-1)]D^3 f_o + \ldots \}$$

$$f''(x) = \frac{1}{h^2}\{D^2 f_o + \frac{1}{6}[(s-2) + (s-1) + (s-2) + s$$

$$+ s + (s-1)]D^3 f_o + \ldots \}$$

For forward difference derivative, at $x = x_o$, $s=0$

$$f''(x) \approx \frac{1}{h^2}\left\{\Delta^2 f_o - \Delta^3 f_o + \Lambda \right\}$$

If we take only one term of the above equation,

$$f''(x_o) \approx \frac{1}{h^2}\left\{f_2 - 2f_1 + f_o\right\}$$

If we take 2 terms from the equation,

$$f''(x_o) \approx \frac{1}{h^2}\{(f_2 - 2 f_1 + f_o) -(f_3 -3 f_2 +3 f_1 - f_o)\}$$

$$\approx \frac{1}{h^2} \{ - f_3 + 4 f_2 - 5 f_1 + 2 f_o \}$$

EXAMPLE 4: HIGHER DERIVATIVES

Estimate $y''(1.7)$ from E.g. 2 using up to D^3 terms and also estimate the associated error.

$$y''(1.7)= \frac{1}{0.2^2} (0.268 - 0.060)$$

$$= 5.200 \text{ (actual answer is } 5.474\text{)}$$

$$Error = \frac{1}{h^2} (\tfrac{11}{12}h^4 \; y^{iv}(x)) \qquad 1.7 \; £ \; x \; £ \; 2.1$$

$$Max.\ Error \quad = 11/12\ \ 0.2^2\ e^{2.3} = \ \ 0.298$$

$$Min.\ Error \quad = 11/12\ 0.2^2\ e^{1.7} \ = \ \ 0.201$$

compared to actual error of 0.274.

2.5 NEWTON-COTES INTEGRATION

. For evenly-spaced data, use Newton-Gregory $P_n\ (x)$.

$n = 1$,

$$\int_{x_o}^{x_1} f(x)\, dx \quad = \quad \int_{x_o}^{x_1} \left(f_o \ + \ s\, \Delta f_o \right) dx$$

$$= \quad h \int_{s=0}^{s=1} \left(f_o \ + \ s\, \Delta f_o \right) ds$$

$$= \quad \left[h\, f_o\, s \ + \ h\, \Delta f_o \ \frac{s^2}{2} \right]_{s=0}^{s=1}$$

$$= \quad h/2\ \ (f_o + f_1)$$

$$Error = \int_{x_o}^{x_1} \frac{s(s-1)}{2} h^2 f''(x)\, dx$$

$$= h^3 f''(x) \int_0^1 \frac{s^2 - s}{2} ds$$

$$= -\frac{1}{12} h^3 f''(x_1)$$

$$x_o < x_1 < x_1$$

Mean value theorem (see A2)

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

$$a \le x \le b$$

This is only true if *g(x)* does not change sign.

In this case,

$$g(x) = \frac{1}{2}(s^2 - s) = \frac{s}{2}(s-1)$$

$$0 \le s \le 1, \; g(x) \le 0$$

For $n = 2$,

$$\int_{x_o}^{x_2} f(x)dx = \int_{x_o}^{x_2} (f_o + s_D f_o + s(s-1)/2\ D^2 f_o)\ dx$$

$$= h \int_o^2 (f_o + s_D f_o + s(s-1)/2\ D^2 f_o)\ ds$$

$$= h\left[f_o\ s + \frac{s^2}{2}\ \Delta\ f_o + \left(\frac{s^3}{6} - \frac{s^2}{4}\right)\Delta^2 f_o \right]_o^2$$

$$= h(2\ f_o + 2_D f_o + 1/3 D^2 f_o)$$

$$= h/3(f_o + 4\ f_1 + f_2)$$

$$Error = -\frac{1}{90} h^5 f^{iv}(x_1)$$

$$where\ x_o < x_1 < x_2$$

Similarly, for $n = 3$, we find that

$$\int_{x_o}^{x_3} f(x)\,dx = \frac{3}{8} h\,(f_o + 3 f_1 + 3 f_2 + f_3)$$

$$Error = -\frac{3}{8} h^5 f^{iv}(x_1) \quad x_o < x_1 < x_3$$

Corollaries:

- for Newton-Cotes formula, error for quadratic interpolation is slightly less than for cubic interpolation.

- errors using $n = 2$ and $n = 3$ are $0(h^5)$, and the coefficients are also similar.

- this suggests that even order rules for Newton-Cotes are especially useful.

In general, Newton-Cotes rules can be written

$$\int_a^b f(x)\,dx \quad » \; w_o\, f(x_o) + w_1\, f(x_1) + w_2\, f(x_2)$$

$$+ \; \ldots \; + w_n\, f(x_n)$$

where w_i = weighting coefficients

$f(x_i)$ = function values at the sampling points.

In summary, Newton-Cotes formulas are:

$n=1$

$$\int_{x_o}^{x_1} f(x)\,dx = h/2\,(f_o + f_1) - 1/12\,h^3 f''(x)$$

¾"Trapezoidal rule"

$n=2$

$$\int_{x_o}^{x_2} f(x)\,dx = h/3(f_o + 4 f_1 + f_2) - 1/90\,h^5 f^{iv}(x)$$

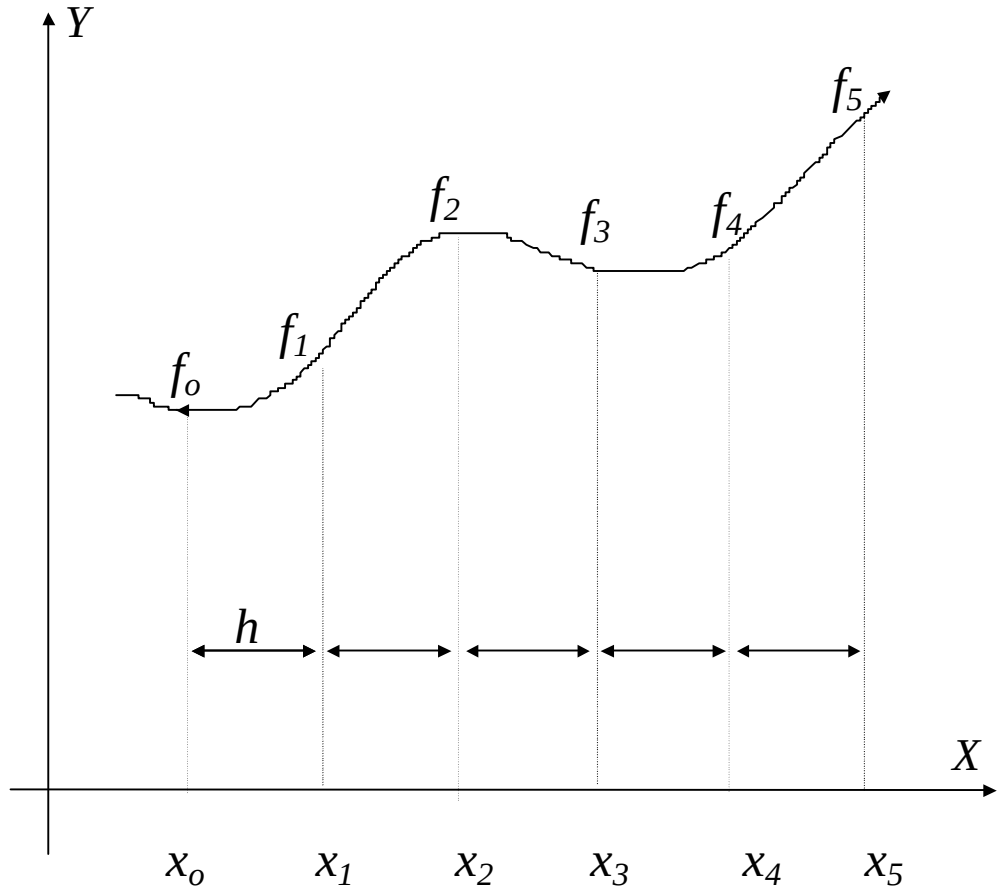
¾ "Simpson ' s 1/3 rule"

$n=3$

$$\int_{x_o}^{x_3} f(x)dx = 3h/8(f_o + 3f_1 + 3 f_2 + f_3) - 3/80\,h^5 f^{iv}(x)$$

¾ "Simpson ' s 3/8 rule"

2.6TRAPEZOIDAL & SIMPSON'S RULES



$$\int_a^b f(x)\,dx = h/2\,(f_0 + 2f_1 + 2f_2 + 2f_3 + 2f_4 + f_5)$$

- simple to compute.
- can be used for unequally spaced values.

EXAMPLE 5: TRAPEZOIDAL RULE

Find the area between $x = 1.8$ and $x = 3.4$.

x	f(x)	x	f(x)
1.6	4.953	2.8	16.445
1.8	6.050	3.0	20.086
2.0	7.389	3.2	24.533
2.2	9.025	3.4	29.964
2.4	11.023	3.6	36.598
2.6	13.664	3.8	44.701

$$\int_{1.8}^{3.4} f(x)\,dx = 0.2/2\,[6.050+2(7.389) + 2(9.025)$$

$$+ \ \ldots \ + \ 29.964]$$

$$= \ 23.9944$$

Recall Local error of Trapezoidal Rule, i.e. error of 1 step

$$= \quad - \frac{1}{12} h^3 f''(x_1) \qquad x_o < x_1 < x_1$$

Global error = $- \frac{1}{12} h^3 [f''(x_1) + f''(x_2) + \ldots + f''(x_n)]$

Since $nh = b - a$, we have

Global error $= - \frac{1}{12} h^3 n \; f''(x)$

$$= \quad - \frac{(b-a)}{12} h^2 f''(x)$$

From Eg. 4 , we have $f(x) = e^x$

$$\int_{1.8}^{3.4} f(x)\, dx = e^{3.4} - e^{1.8} = 23.9144$$

Actual error $= 23.9144 - 23.9944 = -0.08$

Global error $= -\frac{1}{12}(0.2)^3 8 \; e^{1.8} \; (min)$

$= -0.0323 \; (min)$

$= -\frac{1}{12}(0.2)^3 8 \; e^{3.4} \; (max)$

$= -0.1598 \; (max)$

If we do not know $f(x)$, we have to estimate $h^2 f''(x)$ from the second order differences.

But can we improve the accuracy using only the simple Trapezoidal Rule?

EXAMPLE 6 : ROMBERG INTEGRATION

Apply Trapezoidal rule using $h = 0.4$ to Eg. 5.

$$I \approx 0.4/2[6.050 + 2(9.025) + 2(13.464) + 2(20.0860) + 29.964]$$

$$= 24.2328$$

Romberg Integration technique:

$$I = \text{computed value} + \text{error}$$

From Eq.1

$$I = 23.9944 + C(0.2)^2 \qquad C \text{ - constant}$$

From Eq.2

$$I = 24.2328 + C(0.4)^2$$

Solving for the true value I, 4(Eq.1) - (Eq.2)

$$\Rightarrow \quad I \approx 23.9944 + 1/3\,(23.9944 - 24.2328)$$

$$= 23.9149 \text{ (cf to 23.9144 exact)}$$

$$Error = 23.9144 - 23.9149$$

$$= -0.0005 \text{ (cf to -0.08 in Eg. 3)}$$

EXAMPLE 7 : SIMPSON'S RULE

Applying Simpson's Rules to Eg. 5, using $h = 0.2$.

Simpson's 1/3 rule Rules:

$$\int_a^b f(x)\,dx = h/3\,(f_1 + 4f_2 + 2f_3 + 4f_4 + \ldots + f_{n+1})$$

$$-\frac{(b-a)}{180} h^4 f^{iv}(x), \qquad x_1 \le x \le x_{n+1}$$

$$\int_{1.8}^{3.4} f(x)\,dx = 0.2/3\,[6.050 + 4\,(7.389)$$

$$+2(9.025) + 4(11.023) + 2(13.464)$$

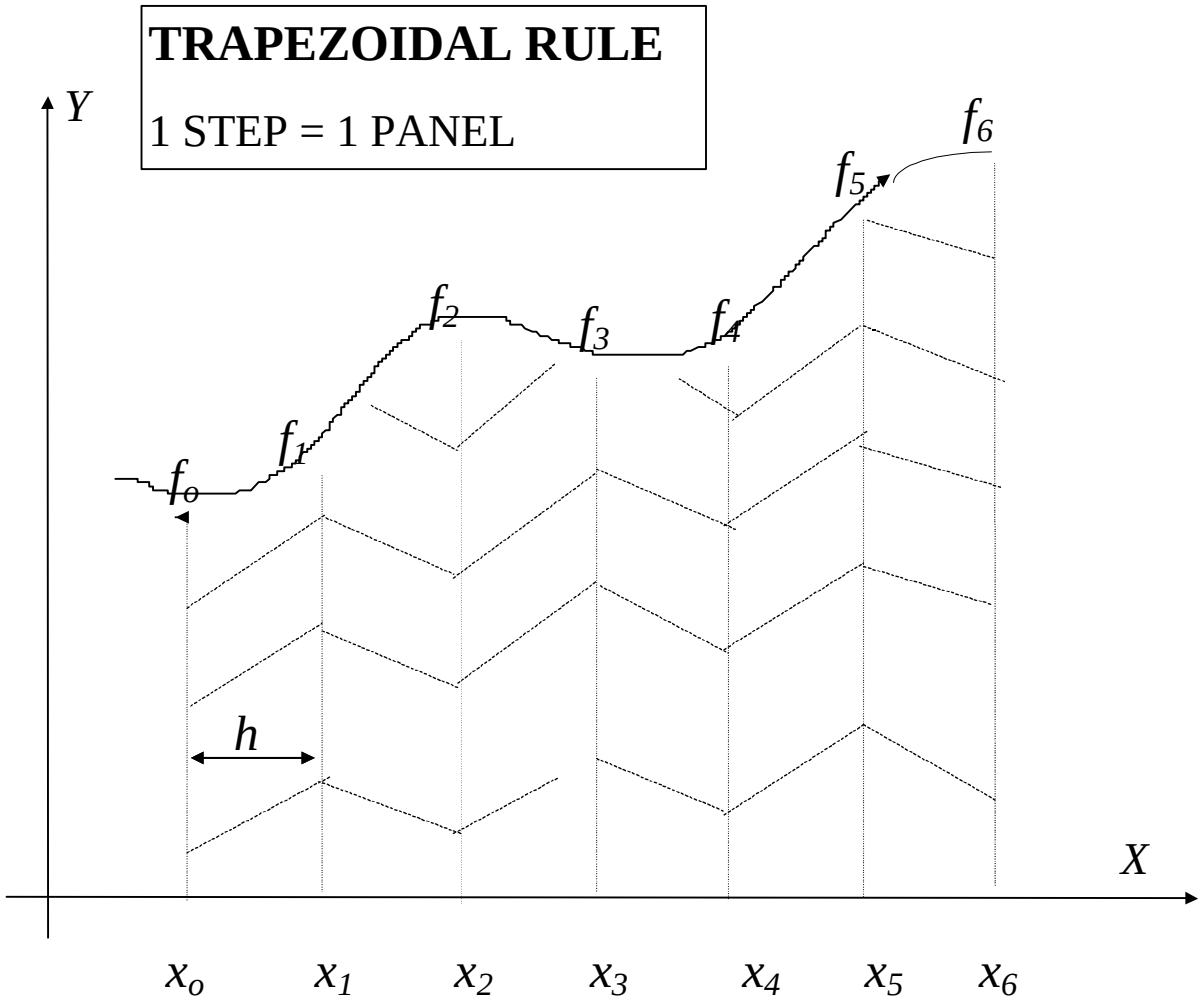
$$+ 4(16.445) + \ldots + 29.964\,] = 23.9149$$

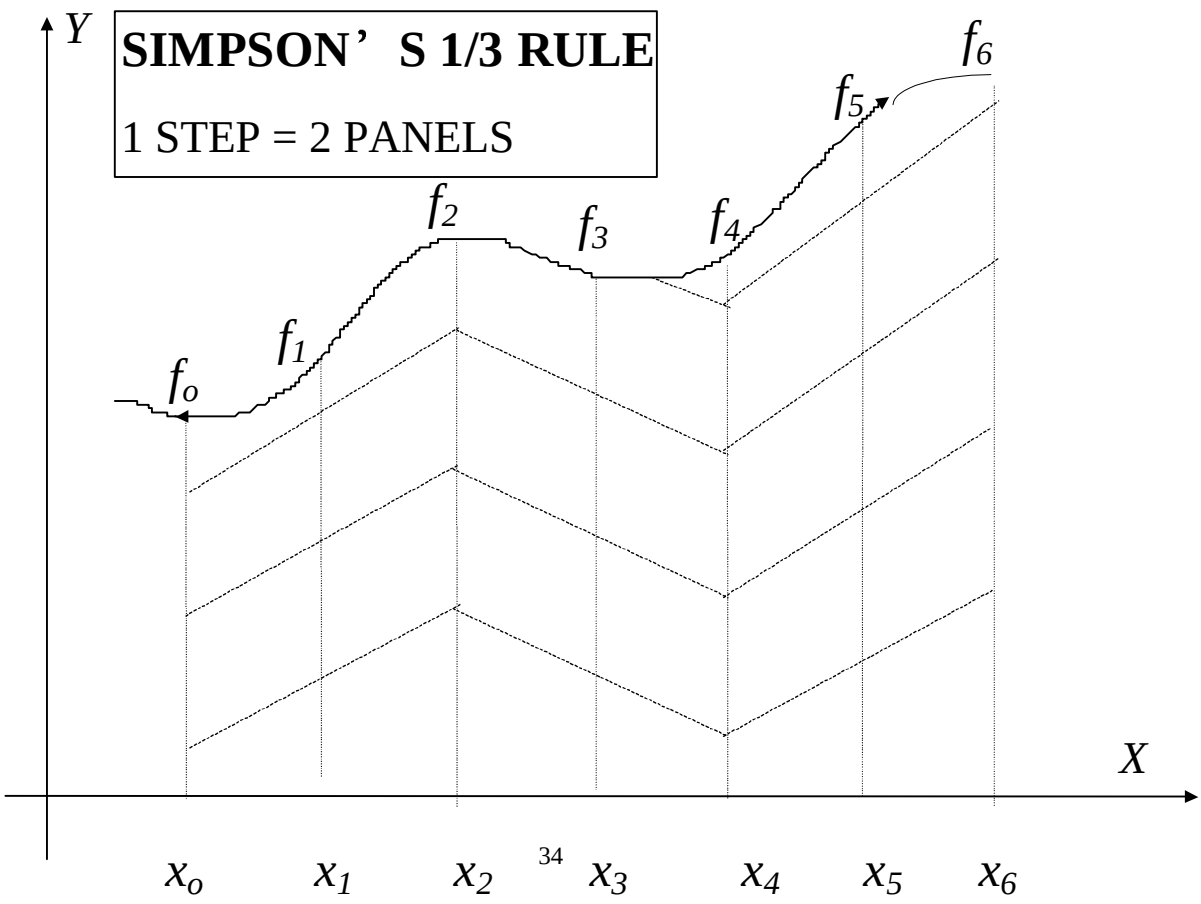
$$Global\ error = -\frac{3.4-1.8}{180}(0.2)^4\ e^{1.8}\ (min)$$

$$= -8.6 \times 10^{-5}\ (min)$$

$$= -\frac{3.4-1.8}{180}(0.2)^4\ e^{3.4}\ (max)$$

$$= -4.3 \times 10^{-4}\ (max)$$


TRAPEZOIDAL RULE
1 STEP = 1 PANEL
Y
X
f_o
f_1
f_2
f_3
f_4
f_5
f_6
h
x_o
x_1
x_2
x_3
x_4
x_5
x_6


SIMPSON' S 1/3 RULE
1 STEP = 2 PANELS
Y
X
f_o
f_1
f_2
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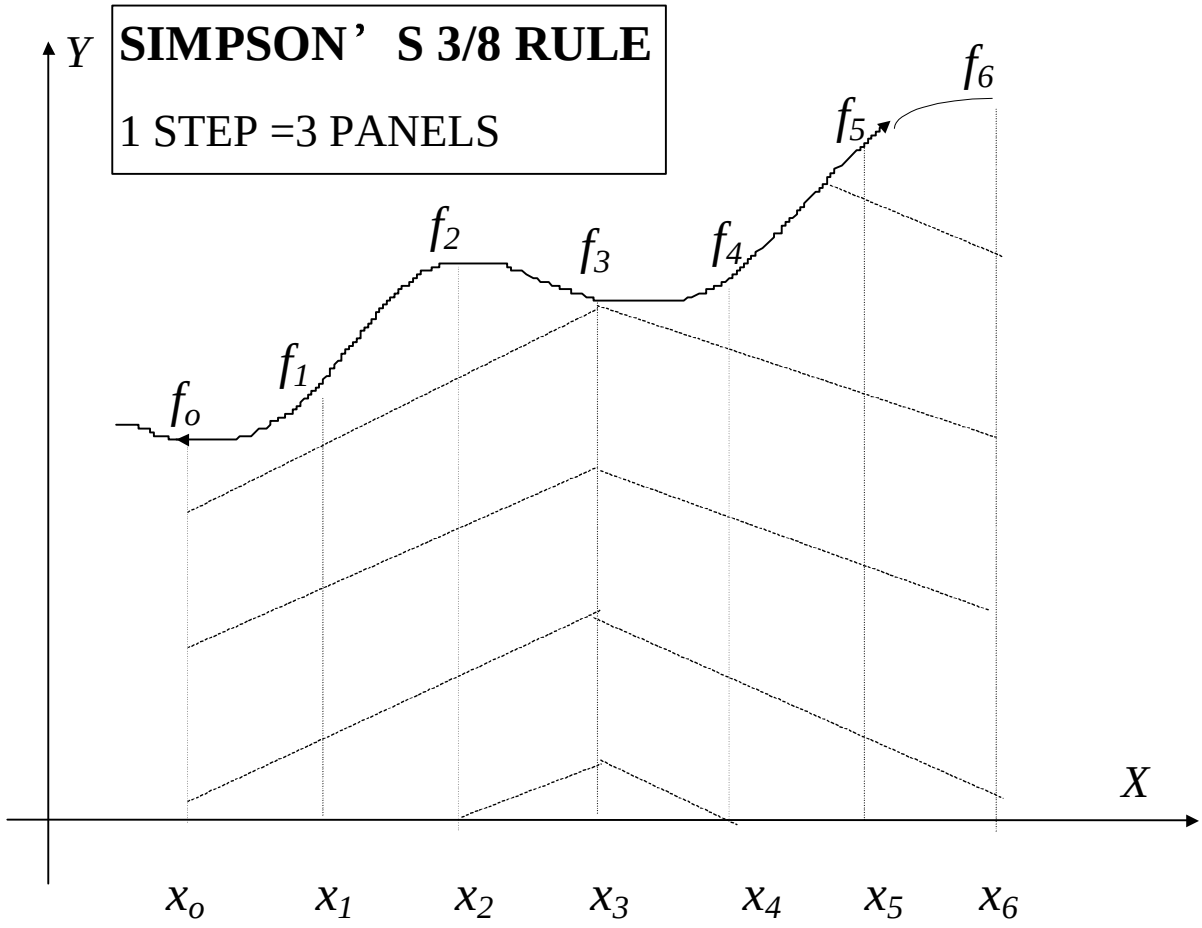

SIMPSON' S 3/8 RULE
1 STEP =3 PANELS
Y
X
f_o
f_1
f_2
f_3
f_4
f_5
f_6
x_o
x_1
x_2
x_3
x_4
x_5
x_6

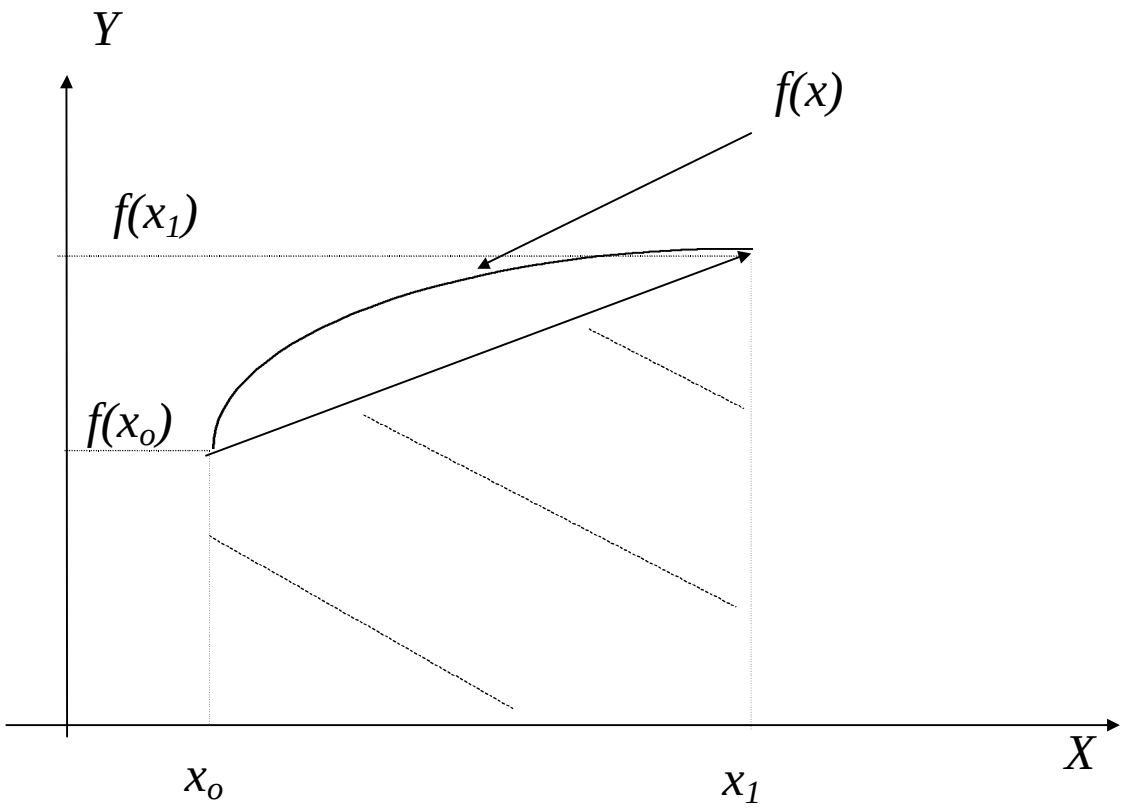
2.7 GAUSSIAN QUADRATURE

Recall Newton-Cotes formula for $n = 1$.

$$\int_a^b f(x)\,dx = h/2\, f(x_o) + h/2\, f(x_1)$$

® *trapezoidal rule*

$$= w_o\, f(x_o) + w_1\, f(x_1)$$



If w_o and w_1 are treated as two unknowns, the above approximation is exact up to degree 1. Similarly, for Newton-Cotes n^{th} degree formula,

$$\int_a^b f(x)\,dx = w_o\, f(x_o) + w_1\, f(x_1) + \ \ldots + \ w_n\, f(x_n)$$

The integration is exact up to $f(x)$ of degree n.

In this case, we have $(n + 1)$ unknowns, i.e. $w_o, w_1, w_2 \ldots w_n$.

Gauss' philosophy to numerical integration is:

"For a given no. of sampling points where in the range of integration should x_i be positioned for ***optimal accuracy****? "*

That is unlike Newton-Cotes**,** Gauss treated w_i and x_i as unknowns, for n^{th} degree polynomial a total of $2(n+1)$ unknown parameters.

Corollaries:

- By suitable positioning of x_i, we can find $2n + 2$ unknowns. This is analogous to fitting Eq. 1 to $2(n+1)$ data points.

- Thus,Gauss' formula is accurate up to degree $2(n) + 1$. Gauss uses integration limits $\pm\ 1$.

(i) 1-point Gaussian $(n = 0)$

$\int_{-1}^{1} f(x)\,dx$ » $w_o\, f(x_o)$

(exact up to degree 1)

Let $f(x) = 1$

$\int_{-1}^{1} 1\,dx = 2 = w_o$

Let $f(x) = x$

$\int_{-1}^{1} x\,dx = 0 = w_o \,.\, x_o$ Þ $x_o = 0$

\ $\int_{-1}^{1} f(x)\,dx$ » $2f(0)$ ¾ mid-point rule.

(ii) 2-point Gaussian *(n = 1)*

$\int_{-1}^{1} f(x)\,dx \;\; » \;\; w_{-1} f(x_{-1}) + w_1 f(x_1)$

(exact up to degree 3)

Let $f(x) = 1$

$$\int_{-1}^{1} 1\,dx = w_{-1}\,1 + w_1\,1 \qquad (1)$$

Let $f(x) = x$

$$\int_{-1}^{1} x\,dx = w_{-1}\,x_{-1} + w_1\,x_1 \qquad (2)$$

Let $f(x) = x^2$

$$\int_{-1}^{1} x^2\,dx = \frac{2}{3} = w_{-1}\,x_{-1}^2 + w_1\,x_1^2 \qquad (3)$$

Let $f(x) = x^3$

$$\int_{-1}^{1} x^3\,dx = 0 = w_{-1}\,x_{-1}^3 + w_1\,x_1^3 \qquad (4)$$

Verify $\int_{-1}^{1} f(x)\,dx \;\; » \;\; 1 f\left(-\frac{1}{\sqrt{3}}\right) + 1 f\left(\frac{1}{\sqrt{3}}\right)$

(iii) 3-point Gaussian *(n = 2)*

$$\int_{-1}^{1} f(x)\,dx \approx w_{-1} f(x_{-1}) + w_o f(x_o) + w_1 f(x_1)$$

(exact for $f(x)$ up to $2n + 1 = 5^{th}$ degree)

Using polynomial substitution, we obtain

$$\int_{-1}^{1} f(x)\,dx = \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right)$$

Corollaries:

. Notice that the sampling points and weights are symmetrical about the mid-point of the range. This type of quadrature is sometimes referred as Gauss -Legendre.

Gaussian Table

n	w_i	x_i
0	2	0
1	1	$\pm$ 0.57735
2	0.88889 0.55556	0 $\pm$ 0.77460
3	0.65214 0.34785	$\pm$ 0.33998 $\pm$ 0.86114
4	0.56889 0.47863 0.23693	0 $\pm$ 0.53847 $\pm$ 0.90618

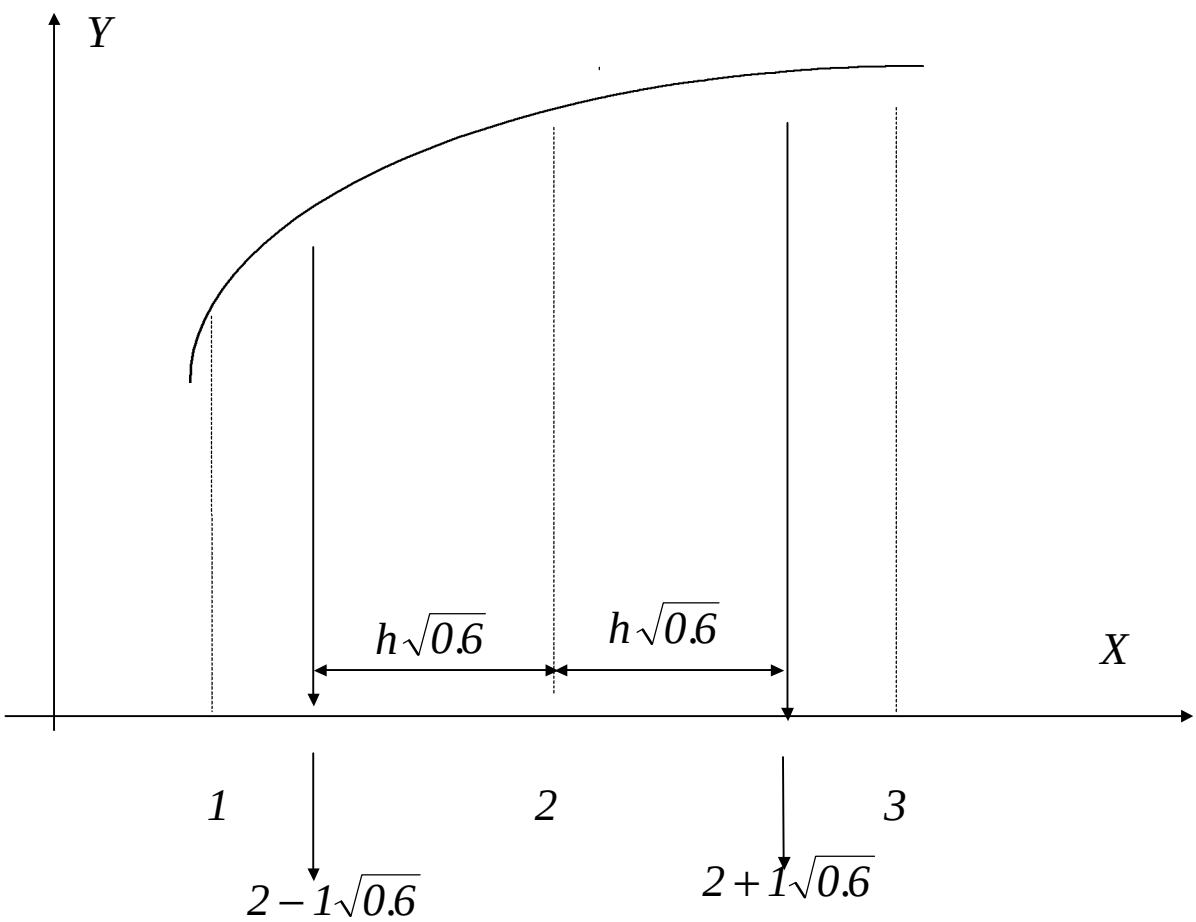
Recall that Gauss integration limits only apply to $\int_{-1}^{1} f(x)\,dx$.

To change the limits of integration, we find the new sampling points by proportioning off on either side of the mid-point of the range.

Weights are also multiplied by halving the range.

EXAMPLE 8: GAUSS' INTEGRATION

Estimate $\int_1^3 f(x)\, dx$ using Gauss' 3 point rule (i.e. $n = 2$).



Range $= 3 - 1 = 2$

Half the range $= h = \dfrac{2}{2} = 1$

$$I = \frac{(3-1)}{2}\left[\frac{5}{9} f\left(2 - 1\sqrt{0.6}\right) + \frac{8}{9} f(2) + \frac{5}{9} f\left(2 + 1\sqrt{0.6}\right)\right]$$

EXAMPLE 9 : GAUSS'S INTEGRATION

Find $\int_0^3 x \cos x \, dx$ using Gauss Table using $n = 2$.

$$\text{Let } f(x) = x \cos x$$

$$f(1.5(1 - \sqrt{0.6})) = f(0.3381) = 0.31896$$

$$f(1.5(1 + \sqrt{0.6})) = f(2.6619) = -2.36147$$

$$f(1.5) = 0.10610$$

$$I = \frac{3}{2}\left[\frac{5}{9}(0.31896) + \frac{8}{9}(0.10610) + \frac{5}{9}(-2.36147)\right]$$

$$I = -1.5606$$

Analytically, from integration by parts,

$$I = \left[x\left(\sin x\right)\right]_o^3 - \int_o^3 \left(\sin x\right) dx$$

$$= 3 \sin 3 + \left[\cos x\right]_o^3$$

$$= 3 \sin 3 + \cos 3 - 1$$

$$= -1.5667$$

EXAMPLE 10 : GAUSS' S INTEGRATION

Double Integrals with variable limits

From Calculus

$$\int_0^1 \int_0^x xe^y \, dy \, dx = \int_0^1 x(e^x - 1) dx$$

$$= \left[xe^x \right]_0^1 - \int_0^1 e^x dx - \frac{1}{2}$$

$$= e^1 - \left[e^x \right]_0^1 - \frac{1}{2}$$

$$= e^1 - \left[e^1 - e^0 \right] - \frac{1}{2}$$

$$= \frac{1}{2}$$

2.8 SUMMARY

Numerical Differentiation → forward difference.

.

Numerical Differentiation → central difference

Numerical Integration →

Newton-Cotes Rule

(n = 0) Mid-point

(n = 1) Trapezoidal

(n = 2) Simpson's 1/3

(n = 3) Simpson's 3/8

(n = 0) $2f(0)$

Gaussian *(n = 1)* → $f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$

Quadrature *(n = 2)* $f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(+\sqrt{\frac{3}{5}}\right)$

Appendix A1:

Proof of $\frac{d}{ds}\binom{s}{n+1} = \binom{s}{n+1}\sum_{1=0}^{n}\frac{1}{(s-i)}$

$$\frac{d}{ds}\binom{s}{n+1} = \frac{d}{ds}\frac{s(s-1)(s-2)\Lambda\ (s-n)}{(n+1)!}$$

$$= \frac{1}{(n+1)!}\frac{d}{ds}\{\ s\ (s-1)(s-2)\ \ldots\ (s-n)\ \}$$

$$= \frac{1}{(n+1)!}\{(s-1)(s-2)\ \ldots\ (s-n)$$

$$+\quad s(s-2)\ \ldots\ (s-n)\ +$$

$$+\quad s(s-1)(s-2)\ \ldots[s-(n-1)]\}$$

$$= \frac{s(s-1)(s-2)\Lambda\ (s-n)}{(n+1)!}\left\{\frac{1}{s} + \frac{1}{s-1} + \frac{1}{s-2} + \Lambda + \frac{1}{s-n}\right\}$$

$$= \binom{s}{n+1}\sum_{i=0}^{n}\frac{1}{(s-i)}$$

At s = 0 ,

$$\frac{d}{ds}\begin{pmatrix} s \\ n+1 \end{pmatrix} = \frac{1}{(n+1)!}\{(-1)\,(-2)\,(-3)\,....\,(-n)\}$$

$$= \frac{(-1)^n\ n!}{(n+1)\ n!}$$

$$= \frac{(-1)^n}{(n+1)}$$

Appendix A2: Mean Value Theorem for Integrals

If $f \in$ C [a,b], $g(x)$ is integrable on $[a,b]$ and $g(x)$ does not change sign on $[a,b]$, then there exists a number c, $a < c < b$, such that

$$\int_a^b f(x)\, g(x)\, dx = f(c) \int_a^b g\ (x)\, dx.$$

TKH 2 Jan 2001