

4. Numerical Integration and Differentiation

4.1 Numerical Integration:

Numerical Integration constitutes a board family of algorithms for calculating the numerical value of a definite integral

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

Why do we need numerical integration?

- To integrate tabulated data

x	0	0.5	1	1.5	2.0
f(x)	1.2	1.8	3.1	4.6	7.6

- Analytical integration may be impossible or infeasible

Such as $\int_0^{\pi} \frac{\sin x}{x} dx$ or $\int_0^2 e^{x^2} dx$

1. Trapezoidal Rule

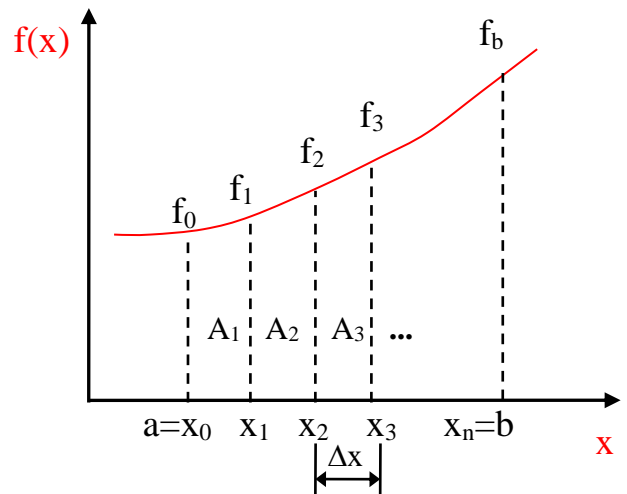
$$\int_a^b f(x) dx$$

n: No. of divisions (strips)

$$\Delta x = \frac{b-a}{n}$$

$$\text{Total area} = \int_a^b f(x) dx = \sum_{i=1}^n A_i$$

$$A_1 = \frac{f_0 + f_1}{2} \cdot \Delta x, \quad A_2 = \frac{f_1 + f_2}{2} \cdot \Delta x, \quad \dots, \quad A_n = \frac{f_{n-1} + f_n}{2} \cdot \Delta x$$



$$\begin{aligned} x_1 &= x_0 + \Delta x \\ &= a + \Delta x \\ x_2 &= x_1 + \Delta x \\ &\dots \end{aligned}$$

$$\int_a^b f(x) dx = \Delta x \left[\frac{f_a}{2} + f_1 + f_2 + \dots + f_{n-1} + \frac{f_b}{2} \right]$$

2. Simpson Rule

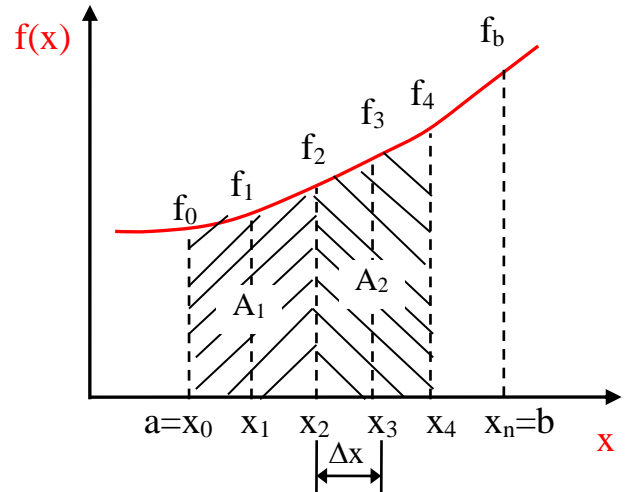
Note: No. of division (strips) should be even

$$A_1 = \frac{\Delta x}{3} (f_0 + 4f_1 + f_2)$$

$$A_2 = \frac{\Delta x}{3} (f_2 + 4f_3 + f_4)$$

⋮

$$A_n = \frac{\Delta x}{3} (f_{n-3} + 4f_{n-2} + f_{n-1})$$



$$\int_a^b f(x) dx = \frac{\Delta x}{3} [f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \dots + 2f_{n-2} + 4f_{n-1} + f_n]$$

$$f_0 = f_a, f_n = f_b, x_1 = x_0 + \Delta x, x_2 = x_1 + \Delta x \dots$$

Ex. Evaluate $I = \int_0^2 e^{-x^2} dx$ using trapezoidal & Simpson methods. take $h = 0.25$.

Sol. No. of division = $\frac{b-a}{h} = \frac{2-0}{0.25} = 8$

n	x_n	Trapezoidal		Simpson		
		$f_n = e^{-x_n^2}$		$f_n = e^{-x_n^2}$		
0	0	1		1		
1	0.25		0.939		0.939	
2	0.5		0.779			0.779
3	0.75		0.570		0.570	
4	1		0.368			0.368
5	1.25		0.210		0.210	
6	1.5		0.105			0.105
7	1.75		0.047		0.047	
8	2	0.018		0.018		
Sums		1.018	3.018	1.018	1.766	1.252

$$(1) \text{ Trapezoidal } I_t = \Delta x \left[\frac{f_0}{2} + f_1 + f_2 + f_3 + f_4 + f_5 + f_6 + f_7 + \frac{f_8}{2} \right]$$

$$= 0.25 \left[\frac{1}{2}(1.018) + 3.018 \right] = 0.88175$$

$$(2) \text{ Simpson } I_s = \frac{\Delta x}{3} [f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + 4f_5 + 2f_6 + 4f_7 + f_8]$$

$$= \frac{0.25}{3} [1.018 + 4 * 1.766 + 2 * 1.252] = 0.88216$$

4.2 Numerical Differentiation:

- **First Order Derivative:** Forward, Backward, Central Difference Formula
- **Second Order Derivative:** Forward, Backward, Central Difference Formula

Why numerical Differentiation needed?

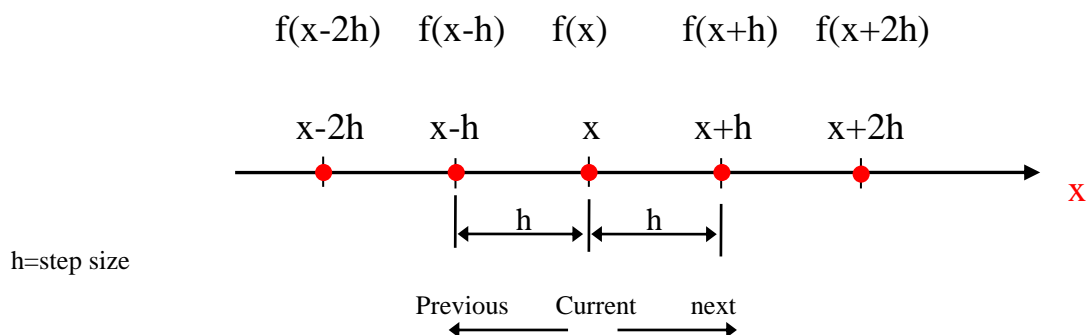
- To diff. tabulated data

x	0	0.5	1	1.5	2.0
f(x)	1.2	1.8	3.1	4.6	7.6

- Analytical Diff. may be more complex

Such as $\frac{d}{dx} \left[\sin(3x^2 + e^{-3x^2}) e^{2x} \right]$ or $\frac{d}{dx} \left[e^{-x^2} \sin(2 \ln(x+1)) \right]$

❖ First Order Derivative



In previous section in finite difference

- **For forward difference** $\Delta f_0 = f_1 - f_0$ In generally $\Delta f_n = f_{n+1} - f_n$

$$\begin{aligned}\Delta^2 f_0 &= \Delta(\Delta f_0) = \Delta f_1 - \Delta f_0 = (f_2 - f_1) - (f_1 - f_0) \\ &= f_2 - 2f_1 + f_0 \\ &\vdots\end{aligned}$$

- **For Backward difference** $\nabla f_1 = f_1 - f_0$ In generally $\nabla f_n = f_n - f_{n-1}$

$$f'(x) = \frac{df}{dx} \approx \frac{\Delta f}{\Delta x} \approx \frac{\Delta f}{h} = \frac{f(x+h) - f(x)}{h}$$

$$f'(x_0) = \frac{1}{h} \Delta f_0 = \frac{f_1 - f_0}{h}$$

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

is called **(2 points forward difference)**

$$f'(x_1) = \frac{1}{h} \nabla f_1 = \frac{f_1 - f_0}{h}$$

$$f'(x) = \frac{f(x) - f(x-h)}{h}$$

is called **(2 points backward difference)**

❖ Using Newton Forward interpolation formula

$$f(x) = f_0 + r\Delta f_0 + \frac{r(r-1)}{2!} \Delta^2 f_0 + \frac{r(r-1)(r-2)}{3!} \Delta^3 f_0 + \dots$$

$$f'(x) = \frac{df}{dx} = \frac{df}{dr} \cdot \frac{dr}{dx}, \quad r = \frac{x - x_0}{h}, \quad \therefore \frac{dr}{dx} = \frac{1}{h}$$

$$\frac{df}{dx} = \frac{1}{h} \cdot \frac{d}{dr} \left[f_0 + r\Delta f_0 + \frac{r(r-1)}{2!} \Delta^2 f_0 + \frac{r(r-1)(r-2)}{3!} \Delta^3 f_0 + \dots \right]$$

$$\therefore f'(x) = \frac{1}{h} \left[\Delta f_0 + \frac{2r-1}{2!} \Delta^2 f_0 + \frac{3r^2-6r+2}{3!} \Delta^3 f_0 + \dots \right]$$

** If Using "Three-point formula" find $f'_0, f'_1,$ and f'_2 .

$$\therefore f'(x) = \frac{1}{h} \left[\Delta f_0 + \frac{2r-1}{2!} \Delta^2 f_0 \right]$$

"Three points formula"

(i) At $x = x_0$ $r = \frac{x_0 - x_0}{h} = 0$

where $r = \frac{x - x_0}{h}$

$$f'(x_0) = f'_0 = \frac{1}{h} \left[\Delta f_0 - \frac{1}{2} \Delta^2 f_0 \right] = \frac{1}{h} \left[\Delta f_0 - \frac{1}{2} \Delta(\Delta f_0) \right] = \frac{1}{h} \left[\Delta f_0 - \frac{1}{2} (\Delta f_1 - \Delta f_0) \right]$$

$$f'_0 = \frac{1}{h} \left[(f_1 - f_0) - \frac{1}{2} ((f_2 - f_1) - (f_1 - f_0)) \right]$$

$$\therefore f'_0 = \frac{1}{2h} [-3f_0 + 4f_1 - f_2]$$

is called **(3 points forward difference)**

$$\therefore f'_x = \frac{1}{2h} [-3f_x + 4f_{x+h} - f_{x+2h}]$$

(ii) At $x = x_1$, $r = \frac{x_1 - x_0}{h} = 1$

$$f'(x_1) = f'_1 = \frac{1}{h} \left[\Delta f_0 + \frac{1}{2} \Delta^2 f_0 \right]$$

$$\therefore f'_1 = \frac{1}{2h} [f_2 - f_0]$$

is called **(3 points central difference)**

$$\therefore f'_x = \frac{1}{2h} [f_{x+h} - f_{x-h}]$$

(iii) At $x = x_2$ $r = \frac{x_2 - x_0}{h} = \frac{2h}{h} = 2$

$$f'_2 = \frac{1}{h} \left[\Delta f_0 + \frac{3}{2} \Delta^2 f_0 \right]$$

$$\therefore f'_2 = \frac{1}{2h} [f_0 - 4f_1 + 3f_2]$$

is called **(3 points backward difference)**

$$\therefore f'_x = \frac{1}{2h} [f_{x-2h} - 4f_{x-h} + 3f_x]$$

Ex. If $f(x) = e^{-x^2} \sin(2\ln(x+1))$, then estimate $f'(2.0)$ using 2-points and 3-points formula. Used the step size, $h=0.2$ and find the absolute error each of them. Which is the best approximation?

Sol. $f(x) = e^{-x^2} \sin(2\ln(x+1))$

x	$f(x) = e^{-x^2} \sin(2\ln(x+1))$
1.6	0.07287
1.8	0.03458
2.0	0.01484
2.2	0.00576
2.4	0.00202

1) **2 points forward difference**

$$f'(x) = \frac{f(x+h) - f(x)}{h} \Rightarrow f'(2.0) = \frac{f(2.2) - f(2.0)}{0.2} = -0.04541$$

2) **2 points backward difference**

$$f'(x) = \frac{f(x) - f(x-h)}{h} \Rightarrow f'(2.0) = \frac{f(2.0) - f(1.8)}{0.2} = -0.09873$$

3) **3 points forward difference**

$$f'_x = \frac{1}{2h} [-3f_x + 4f_{x+h} - f_{x+2h}]$$

$$\therefore f'(2.0) = \frac{1}{2*0.2} [-3f(2.0) + 4f(2.2) - f(2.4)] = -0.05877$$

4) **3 points central difference**

$$\therefore f'_x = \frac{1}{2h} [f_{x+h} - f_{x-h}] \Rightarrow f'(2.0) = \frac{f(2.2) - f(1.8)}{2*0.2} = -0.07207$$

5) **3 points backward difference**

$$f'_x = \frac{1}{2h} [f_{x-2h} - 4f_{x-h} + 3f_x]$$

$$\therefore f'(2.0) = \frac{1}{2*0.2} [f(1.6) - 4f(1.8) + 3f(2.0)] = -0.05237$$

- **To find the absolute error and the best method. We need Exact solution for the derivative for x=2.0**

$$f(x) = e^{-x^2} \sin(2 \ln(x+1))$$

$$\frac{df}{dx} = f'(x) = e^{-x^2} \left[\frac{2}{x+1} \cos(2 \ln(x+1)) \right] - 2xe^{-x^2} \sin(2 \ln(x+1))$$

$$\therefore f'(2.0) = -0.06651 \quad \text{Exact solution}$$

Absolute error, $\varepsilon = |Exact\ value - Numerical\ value|$

No.	Method	Numerical value	Exact	Absolute error
1	2 points forward difference	-0.04541	-0.06651	0.02110
2	2 points backward difference	-0.09873	-0.06651	0.03222
3	3 points forward difference	-0.05877	-0.06651	0.00774
4	3 points central difference	-0.07207	-0.06651	0.00556
5	3 points backward difference	-0.05237	-0.06651	0.01414

The best approximation method is **3 point central difference** since min. error

H.W. find $f'_0, f'_1,$ and f'_2 using four-point formula.

N.B. if h not constant using Lagrange interpolation to find differentiations.

$$f(x) = \sum_{k=0}^n N_k(x) f_k, \quad \text{where } N_k(x) = \prod_{\substack{j=0 \\ j \neq k}}^n \frac{(x - x_j)}{(x_k - x_j)}$$