Lecture 30: Numerical Integration – Simpson's rule

(09-Oct-2012)

LECTURE - 30

9/10/2012

Newton - Cotes Integration Formulas

Yesterday, we have seen that numerical integration can be achieved through Newton - Cotes formulas.

$$I = \Delta x \int_0^s P_n(s)\, ds$$

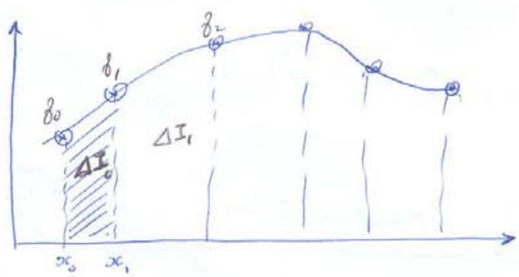
Based on the degree of the Newton's forward difference polynomial, you will get different types of Newton Cotes formulas.

1) When $n = 0$ $\longrightarrow$ Rectangular Formula

$$\underline{\underline{I = C s \Delta x}}$$

2) When $n = 1$ $\longrightarrow$ Trapezoid Formula

$$\Delta I_i = \frac{\Delta x}{2}\left[f_i + f_{i+1}\right]$$



$$I = \Delta I_0 + \Delta I_1 + \cdots + \Delta I_{n-1}$$

i.e. $$I = \sum_{i=0}^{n-1} \Delta I_i = \frac{1}{2}\sum_{i=0}^{n-1} \Delta x_i \left[f_i + f_{i+1}\right]$$

$\Rightarrow$ For equally spaced data

$$\boxed{I = \frac{1}{2}\Delta x\left[f_0 + 2f_1 + 2f_2 + \cdots + 2f_{n-1} + f_n\right]}$$

This is the famous trapezoid rule for integration.

When you evaluated

$$\Delta I_i = \frac{1}{2}\Delta x\left[f_i + f_{i+1}\right]$$

or $\Delta I_0 = \frac{1}{2}\Delta x\left[f_0 + f_1\right]$

⇒ The error in integration is:

$$\text{Error} = \Delta x \int_0^1 \frac{s(s-1)}{2}\Delta x^2 f''(\xi)\,ds$$

$$= -\frac{1}{12}\Delta x^3 f''(\xi) \qquad \left(\text{i.e. of } O(\Delta x^3)\right)$$

⇒ The total error for full integration:

$$\text{Total error} = \sum_{i=0}^{n-1} \text{Error}_i = \sum_{i=0}^{n-1}\left[-\frac{1}{12}\Delta x^3 f''(\xi)\right]$$

$$= -\frac{n}{12}\Delta x^3 f''(\xi) = \frac{(x_n - x_0)}{\Delta x}\cdot\frac{1}{12}\Delta x^3 f''(\xi)$$

i.e. $\text{Error} \rightarrow O(\Delta x^2)$

<u>When $n = 2$ for $P_n(s)$ in Newton-Cotes</u>

$$I = \Delta x \int_0^s P_n(s)\,ds$$

When $n = 2$ (i.e second degree polynomial).
you require two increments and data points x_0, x_1, x_2 for one interval of the polynomial

∴ The integration has to be from x_0 to x_2.

Or $s = 0$ to $s = \frac{x_2 - x_0}{\Delta x} = \underline{\underline{2}}$

Then

$$\Delta I = \Delta x \int_0^2 \left[y_0 + s\,\Delta y_0 + \frac{s(s-1)}{2}\,\Delta^2 y_0 \right] ds$$

$$= \Delta x \left[y_0 s + \frac{s^2}{2}\Delta y_0 + \frac{1}{2}\left(\frac{s^3}{3} - \frac{s^2}{2}\right)\Delta^2 y_0 \right]_0^2$$

$$= \Delta x \left[2y_0 + 2(y_1 - y_0) + \frac{4}{2}\left(\frac{2}{3} - \frac{1}{2}\right)(y_2 - 2y_1 + y_0) \right]$$

$$= \Delta x \left[\cancel{2y_0} + 2y_1 - \cancel{2y_0} + \frac{1}{3}y_2 - \frac{2}{3}y_1 + \frac{1}{3}y_0 \right]$$

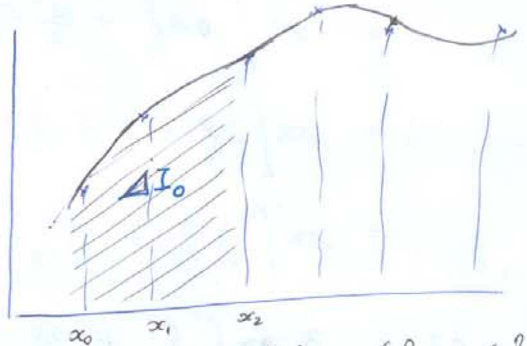
$$= \Delta x \left[\frac{1}{3}y_2 + \frac{4}{3}y_1 + \frac{1}{3}y_0 \right] = \underline{\frac{\Delta x}{3}\left[y_2 + 4y_1 + y_0 \right]}$$

This is the Simpson's $\frac{1}{3}$rd rule for evaluating integral of one interval of second degree polynomial in Newton Cotes.

$$\text{i.e.} \quad \Delta I_0 = \frac{\Delta x}{3}\left[y_2 + 4y_1 + y_0 \right]$$

For the entire integral

Also note that the number of increments should be even.



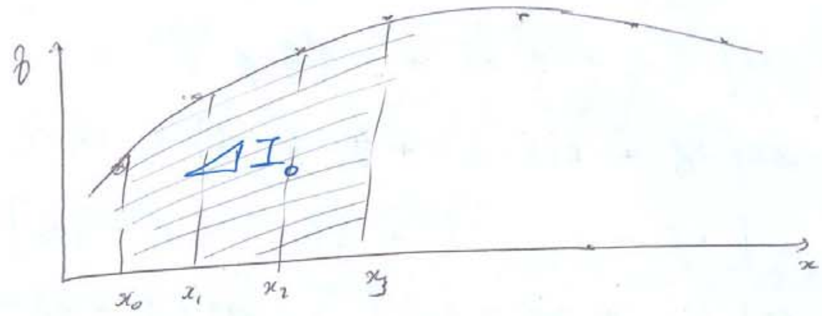
$$I = \frac{\Delta x}{3}\Big[(y_0 + 4y_1 + y_2) + (y_2 + 4y_3 + y_4) + (y_4 + 4y_5 + y_6) + \cdots + (y_{n-2} + 4y_{n-1} + y_n)\Big]$$

$$= \frac{\Delta x}{3}\left[y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + \cdots \right]$$

This is Simpson's $\frac{1}{3}$rd rule for evaluating integration.

→ I request you to self study the order of error for one interval as well as for entire integral.

When $n = 3$ for $P_n(s)$ in Newton-Cotes



$$\Delta I = \Delta x \int_0^s P_n(s)\, ds \qquad \text{the data points } x_0, x_1, x_2, x_3 \quad s = 3$$

$$= \Delta x \int_0^3 \left(y_0 + s \Delta y_0 + \frac{s(s-1)}{2} \Delta^2 y_0 + \frac{s(s-1)(s-2)}{3!} \Delta^3 y_0 \right) ds$$

$$= \Delta x \left[s y_0 + \frac{s^2}{2} \Delta y_0 + \left(\frac{s^3}{6} - \frac{s^2}{4} \right) \Delta^2 y_0 + \left(\frac{s^4}{24} - \frac{s^3}{6} + \frac{s^2}{6} \right) \Delta^3 y_0 \right]_0^3$$

$$= \Delta x \left[3 y_0 + \frac{9}{2}(y_1 - y_0) + \frac{9}{4}(y_2 - 2y_1 + y_0) + \frac{3}{8}(y_3 - 3y_2 + 3y_1 - y_0) \right]$$

$$= \Delta x \left[\frac{3}{8} y_3 + \frac{9}{8} y_2 + \frac{9}{8} y_1 + \frac{3}{8} y_0 \right]$$

$$\Delta I = \frac{3}{8} \Delta x \left[y_0 + 3y_1 + 3y_2 + y_3 \right]$$

This is Simpson's $\frac{3}{8}$ th rule for integration.

$\Rightarrow$ The whole integration can be given by:

$$I = \frac{3}{8} \Delta x \left[y_0 + 3y_1 + 3y_2 + 2y_3 + 3y_4 + 3y_5 + 2y_6 + \cdots + 3y_{n-1} + y_n \right]$$

(Provided the total number of increments are multiple of three.)

You can identify the order of local and global error for Simpson's $\frac{3}{8}$ rule.

Higher-order Newton-Cotes Formulas

As you are aware: $I = \int_a^b f(x)\,dx \cong \Delta x \int_0^s P_n(s)\,ds$

Incorporating higher order polynomials, we can get higher order expressions for N-C formulas.

~~$I = \Delta x \int$~~

Solution to Yesterday's quiz question:

Find the expression for IVth order centered difference formula for second derivative of a function $f(x)$ at any point $x = x_i$

Note, let the data set be (equally spaced Δx)

x	f	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$
x_0	f_0				
		$f_1 - f_0$			
x_1	f_1		$f_2 - 2f_1 + f_0$		
		$f_2 - f_1$		$f_3 - 3f_2 + 3f_1 - f_0$	
x_2	f_2		$f_3 - 2f_2 + f_1$		$f_4 - 4f_3 + 6f_2 - 4f_1 + f_0$
		$f_3 - f_2$		$f_4 - 3f_3 + 3f_2 - f_1$	
x_3	f_3		$f_4 - 2f_3 + f_2$		
		$f_4 - f_3$		$f_5 - 3f_4 + 3f_3 - f_2$	
x_4	f_4		$f_5 - 2f_4 + f_3$		
		$f_5 - f_4$		$f_6 - 3f_5 + 3f_4 - f_3$	
x_5	f_5		$f_6 - 2f_5 + f_4$		
		$f_6 - f_5$			
x_6	f_6				

$$P_n''(x) = \frac{1}{\Delta x^2}\left[\Delta^2 f_0 + (s-1)\Delta^3 f_0 + \frac{6s^2 - 18s + 11}{12}\Delta^4 f_0 + \cdots\right]$$

We want a fourth degree polynomial approximation. Therefore, the expression for $P_n''(x)$ can be truncated after $\Delta^4 f_0$ term.

A centered difference for the second derivative in fourth order is required. As evident from forward difference table the data points involved for $\Delta^4 f_0$ are f_0, f_1, f_2, f_3, and f_4.

$\Rightarrow$ Therefore it is prudent to take $x = x_2$ as the point of interest for finding second derivative as it centers the range from x_0 to x_4.

$\Rightarrow \therefore x = x_2$ and hence $s = \dfrac{x_2 - x_0}{\Delta x} = 2$

$$\therefore P_n''(x_2) = \frac{1}{\Delta x^2}\left[\Delta^2 f_0 + \Delta^3 f_0 - \frac{1}{12}\Delta^4 f_0\right] + \text{error}.$$

$$= \frac{1}{\Delta x^2}\left[(f_2 - 2f_1 + f_0) + (f_3 - 3f_2 + 3f_1 - f_0) - \frac{1}{12}(f_4 - 4f_3 + 6f_2 - 4f_1 + f_0)\right]$$

$$= \frac{-f_4 + 16f_3 - 30f_2 + 16f_1 - f_0}{12\Delta x^2}$$

$\therefore$ At any point $x = x_i$,

$$\left.\frac{d^2 f}{dx^2}\right|_i = \frac{-f_{i+2} + 16f_{i+1} - 30f_i + 16f_{i-1} - f_{i-2}}{12\Delta x^2}$$