

CE 601: Numerical Methods

Lecture 21

Numerical Integration

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Numerical Integration

- For a given set of discrete data (x_i, f_i) , we have seen that we can develop a function relation of 'f' w.r.t. 'x' using polynomial approximations.

→ We also said that such polynomials should be able to do

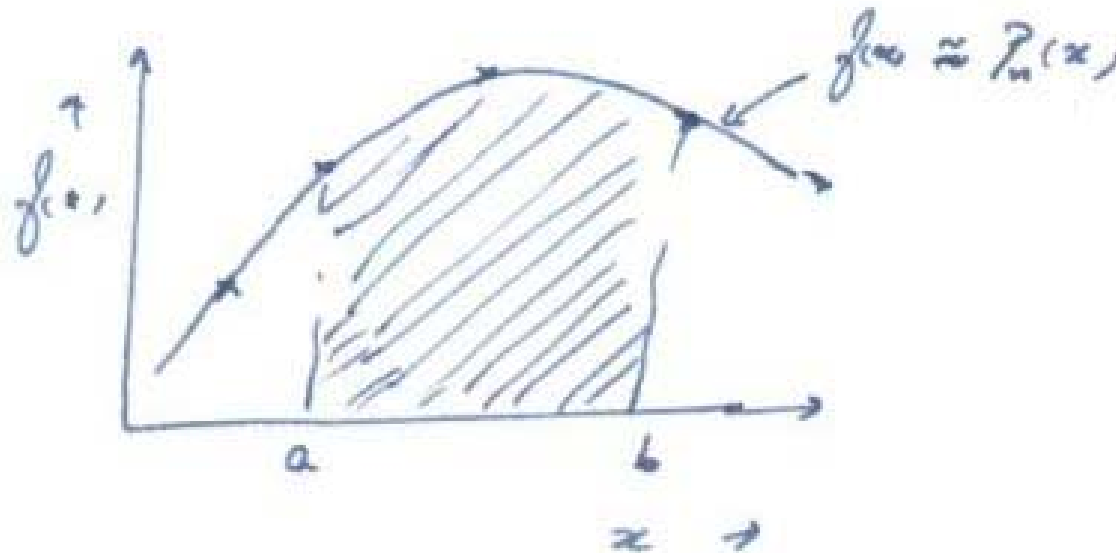
- ❖ Interpolation (already seen)
- ❖ Differentiation (numerical differentiation)
- ❖ Integration

→ The numerical integration schemes will be discussed here.

- If we want to do, $I = \int_a^b f(x)dx$

Then bound on the data set, we had formed

$$f(x) \approx P_n(x), \therefore I = \int_a^b f(x)dx \approx \int_a^b P_n(x)dx.$$



- How the polynomials are constructed, you have already seen.

- Using direct-fit polynomials

$$I = \int_a^b f(x)dx \approx \int_a^b P_n(x)dx = \int_a^b (a_0 + a_1x + \cdots + a_nx^n)dx$$

- Similarly Lagrange polynomials, Divided difference, Newton's polynomials, etc. can be integrated.

- The evaluation of integrals of functions using such polynomials are called quadratures.

- Newton – Cotes Quadratures

Recall the Newton's forward difference polynomial for uniformly spaced data

$$P_n(x) = f_0 + s\Delta f_0 + \frac{s(s-1)}{2!}\Delta^2 f_0 + \cdots + \frac{s(s-1)(s-2)\cdots(s-(n-1))}{n!}\Delta^n f_0$$

$$\left[\text{Error} = \frac{s(s-1)(s-2)\cdots(s-n)}{(n+1)!}(\Delta x)^{n+1} f^{n+1}(\xi); x_0 \leq x \leq x_n \right]$$

$$\therefore I = \int_a^b f(x)dx \approx \int_a^b P_n(x)dx$$

$$s = \frac{x - x_0}{\Delta x} \quad \text{or, } x = x_0 + s\Delta x$$

$$\text{For } x = a, \quad a = x_0 + s(a)\Delta x$$

$$x = b, \quad b = x_0 + s(b)\Delta x.$$

$$I \approx \Delta x \int_{s(a)}^{s(b)} P_n(s)ds.$$

If we choose the base point of the polynomial at $x = a$,

then $s = 0$ at $x = a$, and $s = \frac{x - a}{\Delta x}$

at $x = b$, $s = \frac{b - a}{\Delta x}$

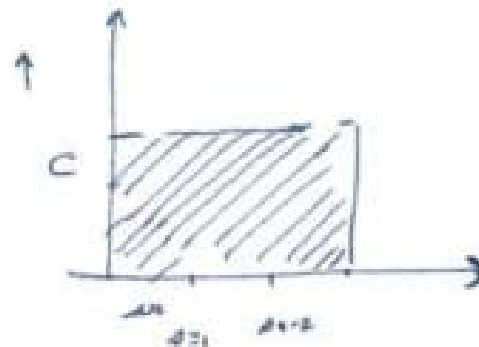
$$\therefore I \approx \Delta x \int_0^s P_n(s) ds.$$

We can adopt various degrees of polynomials for our convenience.

1) If $n = 0$,

then $I = \Delta x \int_0^s P_0(s) ds$

$P_0 \rightarrow$ Some constant C ,



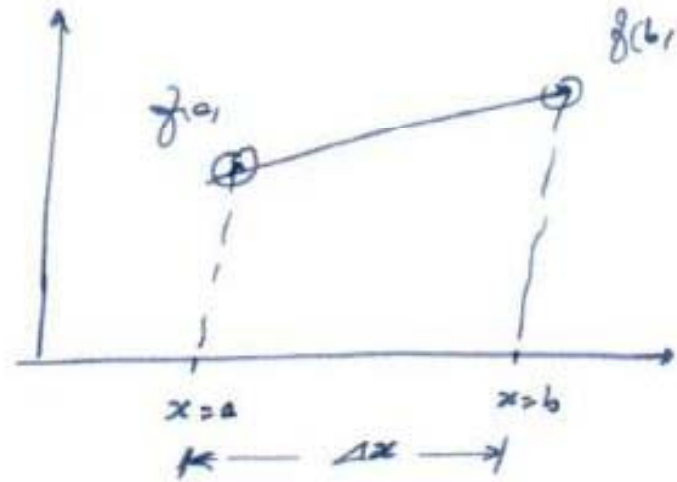
$I = \Delta x C s$ This is rectangular formula for numerical integration.

2) If $n = 1$

$$I = \Delta x \int_0^s P_1(s) ds$$

$$= \Delta x \int_0^s (f_0 + s \Delta f_0) ds$$

$$= \Delta x \left[s f_0 + \frac{s^2}{2} \Delta f_0 \right]$$



So if your data set is such a way that you used a first degree polynomial between $x = a$ and $x = b$ and if they are two consecutive points, Then at $x = a$, $s = 0$

$$x = b, s = 1, \text{ then: } I = \Delta x \int_0^1 P_1(s) ds$$

$$\therefore I = \Delta x \left[f_0 + \frac{1}{2} \Delta f_0 \right]$$

$$= \Delta x \left[f_0 + \frac{1}{2} (f_1 - f_0) \right]$$

$$I = \frac{\Delta x}{2} [f_0 + f_1] \rightarrow \text{This is trapezoidal rule to find area or integration,}$$

If linear splines are used to connect data from $x = x_0$ to $x = x_n$

In such situations, the integration $I = \int_{x_0}^{x_n} f(x)dx$ will

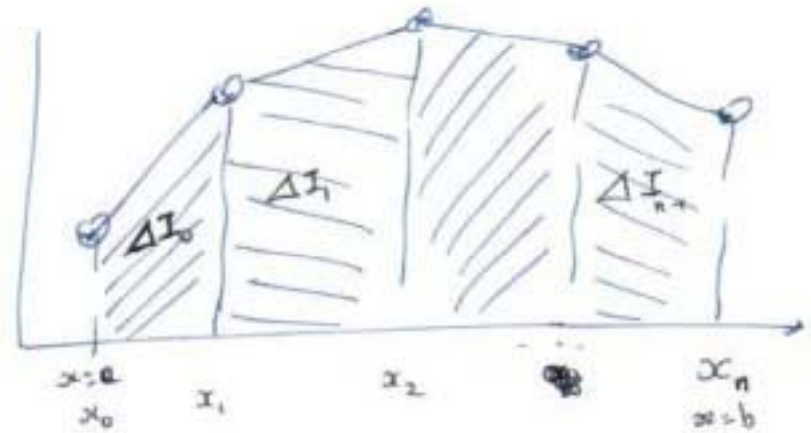
be summations $I \approx \Delta I_0 + \Delta I_1 + \cdots + \Delta I_{n-1}$

$$\text{Now } \Delta I_0 = \frac{\Delta x}{2}(f_0 + f_1)$$

$$\text{Similarly, } \Delta I_1 = \frac{\Delta x}{2}(f_1 + f_2)$$

$$\therefore I = \sum_{i=0}^{n-1} \Delta I_i = \frac{1}{2} \sum_{i=0}^{n-1} \Delta x [f_i + f_{i+1}]$$

$$\text{i.e. } \boxed{I = \frac{1}{2} \Delta x [f_0 + 2f_1 + 2f_2 + \cdots + 2f_{n-1} + f_n]} \rightarrow \text{Trapezoidal Rule}$$



Q. What will be the order of approximation error for this trapezoidal rule?

$$\text{Error for a single interval say } \Delta I_i, E_i = \Delta x \int_0^1 \left[\frac{s(s-1)}{2} \Delta^2 f_0 + \dots \right] ds$$

$$\begin{aligned} \text{i.e. } E_i &= \Delta x \int_0^1 \frac{s(s-1)}{2} \Delta x^2 f''(\zeta) ds \\ &= -\frac{1}{12} \Delta x^3 f''(\zeta) \rightarrow O(\Delta x^3) \end{aligned}$$

$$\text{For } I = \sum \Delta I_i$$

$$\begin{aligned} \text{Total error} &= \sum_{i=0}^{n-1} E_i = \sum_{i=0}^{n-1} \left[-\frac{1}{12} \Delta x^3 f''(\zeta) \right] \\ &= -\frac{n}{12} \Delta x^3 f''(\zeta) \\ &= -\left(\frac{x_n - x_0}{\Delta x} \right) \frac{1}{12} \Delta x^3 f''(\zeta) \rightarrow O(\Delta x^2) \end{aligned}$$

That is, total integration is of $O(\Delta x^2)$

3) When $n = 2$ for Newton-Cotes integration

$$\text{Recall } I = \Delta x \int_0^s P_n(s) ds$$

If $n = 2$, then second degree polynomial.

Minimize three points required.

If we choose three consecutive points $x = a = x_0, x = x_1, x = b = x_2$,
for $P_2(s)$ development, then at $x = a = x_0, s = 0$

at $x = x_1, s = 1$

at $x = b = x_2, s = 2$.

$$\therefore I = \Delta x \int_0^2 \left[f_0 + s \Delta f_0 + \frac{s(s-1)}{2} \Delta^2 f_0 \right] ds$$

$$\begin{aligned}
I &= \Delta x \left[sf_0 + \frac{s^2}{2} \Delta f_0 + \frac{1}{2} \left(\frac{s^3}{3} - \frac{s^2}{2} \right) \Delta^2 f_0 \right]_0^2 \\
&= \Delta x \left[2f_0 + 2(f_1 - f_0) + \frac{4}{2} \left(\frac{2}{3} - \frac{1}{2} \right) (f_2 - 2f_1 + f_0) \right] \\
&= \Delta x \left[\frac{1}{3} f_2 + \frac{4}{3} f_1 + \frac{1}{3} f_0 \right] \\
\boxed{I = \frac{\Delta x}{3} [f_2 + 4f_1 + f_0]} &\rightarrow \text{Simpson's } \frac{1}{3}^{\text{rd}} \text{ rule.}
\end{aligned}$$

→ This is only applied only for 1 interval between x_0 and x_2 .

→ If there are many intervals (especially while using splines),

$$I = \Delta I_0 + \Delta I_1 + \cdots + \Delta I_n$$

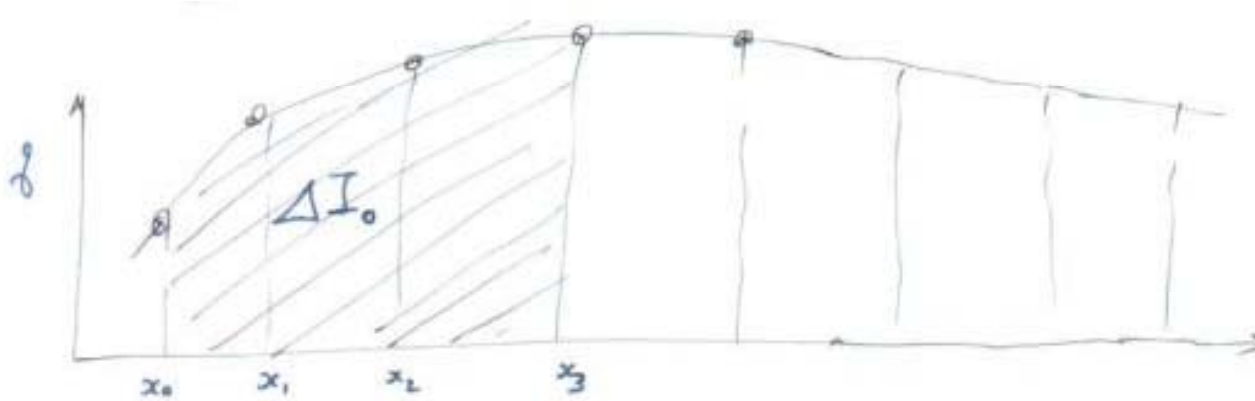
$$= \frac{\Delta x}{3}(f_0 + 4f_1 + f_2) + \frac{\Delta x}{3}(f_2 + 4f_3 + f_4) + \cdots + \frac{\Delta x}{3}(f_{n-2} + 4f_{n-1} + f_n)$$

$$I = \frac{\Delta x}{3}[f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots]$$

→ The number of data points should be odd and minimum 3.

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

4) When $n = 3$



$$\Delta I_0 = \Delta x \int_0^s P_3(s) ds$$

$$= \Delta x \int_0^3 \left(f_0 + s \Delta f_0 + \frac{s(s-1)}{2} \Delta^2 f_0 + \frac{s(s-1)(s-2)}{6} \Delta^3 f_0 \right) ds$$

$$= \Delta x \left[s f_0 + \frac{s^2}{2} \Delta f_0 + \left(\frac{s^3}{6} - \frac{s^2}{4} \right) \Delta^2 f_0 + \left(\frac{s^4}{24} - \frac{s^3}{6} + \frac{s^2}{6} \right) \Delta^3 f_0 \right]_0^3$$

$$= \Delta x \left[\frac{3}{8} f_3 + \frac{9}{8} f_2 + \frac{9}{8} f_1 + \frac{3}{8} f_0 \right]$$

$$\boxed{\Delta I_0 = \frac{3}{8} \Delta x [f_0 + 3f_1 + 3f_2 + f_3]} \rightarrow \text{Simpson's } \frac{3}{8}^{\text{th}} \text{ rule for numerical integration.}$$

So Total integration for $(n + 1)$ data points using

Simpson's $\frac{3}{8}$ th rule will be,

$$I = \Delta I_0 + \Delta I_1 + \cdots + \Delta I_n$$

$$= \frac{3}{8} \Delta x [f_0 + 3f_1 + 3f_2 + 2f_3 + 3f_4 + 3f_5 + 2f_6 + \cdots + 3f_{n-1} + f_n]$$

→ The number of increments here should be multiples of three.

→ Total data points = $4 + 3k$; where $k \rightarrow$ No. of intervals.

→ The local and global error order can be inferred appropriately.