Lecture 29: **Numerical Integration**

(08-Oct-2012)

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08-OCT-2012

Difference Formulas using Taylor's Series

As discussed in the last class, you can write a function in terms of Taylor's series with infinite terms.

Say at $x = x_0$, if $f(x) = f_0$ is known to you, then for any other value of $x \neq x_0$ and $x - x_0 = \Delta x$, we can define $f(x)$

$$f(x) = f_0 + f_0' \Delta x + \frac{1}{2!} f_0'' \Delta x^2 + \dots + \frac{1}{n!} f_0^{(n)} \Delta x^n + \dots$$

or

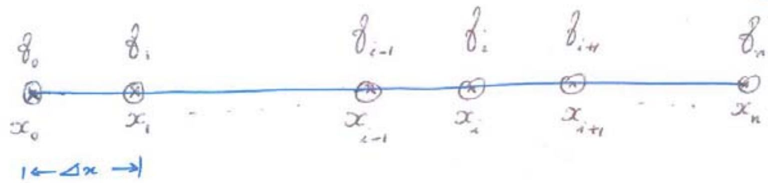
$$f(x) = f_0 + \frac{1}{1!} f_0' \Delta x + \frac{1}{2!} f_0'' \Delta x^2 + \dots + \frac{1}{n!} f_0^{(n)} \Delta x^n + R^{(n+1)}$$

where $$R^{(n+1)} = \frac{1}{(n+1)!} f^{(n+1)}(\xi) \, \Delta x^{n+1}$$

$$x_0 \le \xi \le x_0 + \Delta x$$

For the discrete data set (x_i, f_i), we can suggest the data line as such (Assuming equally spaced data):

x_i	f_i
x_0	f_0
x_1	f_1
x_2	f_2
$\vdots$	$\vdots$
x_n	f_n



Now keeping at $x = x_i$, $f(x) = f(x_i) = f_i$ as base point, the Taylor's series at $x_i + \Delta x$ is given as

$$f(x_i + \Delta x) = f_{i+1} = f_i + f_i' \Delta x + \frac{1}{2!} f_i'' \Delta x^2 + \frac{1}{6} f_i^{(III)} \Delta x^3 + \cdots + \cdots + \frac{1}{n!} f_i^{(n)} \Delta x^n + \cdots$$

Similarly

$$f(x_i - \Delta x) = f_{i-1} = f_i - f_i' \Delta x + \frac{1}{2!} f_i'' \Delta x^2 - \frac{1}{6} f_i^{(3)} \Delta x^3 + \cdots$$

Now evaluate

$$f_{i+1} - f_{i-1} = 2 f_i' \Delta x + \frac{1}{3} f_i^{(3)} \Delta x^3 + \cdots$$

Truncating the series from $f_i^{(3)}$ terms, we get:

$$f_i' = \left.\frac{df}{dx}\right|_{x_i} = \frac{f_{i+1} - f_{i-1}}{2\Delta x} - \frac{1}{6} f_i^{(3)}(\xi) \Delta x^2$$

Again

$$f_{i+1} + f_{i-1} = 2 f_i + f_i^{(II)} \Delta x^2 + \frac{1}{12} f_i^{(4)} \Delta x^4 + \cdots$$

Truncating from $f_i^{(4)}$ term:

$$f_{i+1} - 2f_i + f_{i-1} = f_i^{(II)} \Delta x^2 + \frac{1}{12} f_i^{(4)}(\xi) \Delta x^4$$

i.e. $$f_i^{(II)} = \left.\frac{d^2 f}{dx^2}\right|_i = \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} + \frac{1}{12} f^{(4)}(\xi) \Delta x^2$$

NUMERICAL INTEGRATION

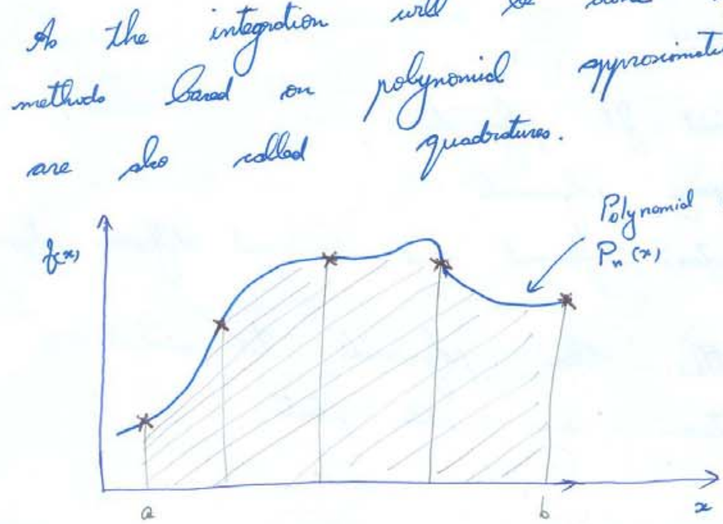
In the beginning, it was told to you that for a given set of discrete data points $(x_i, f(x_i))$, you can make a polynomial approximation for the function $f(x)$,

i.e $f(x) \approx P_n(x)$.

This polynomial approximation can be used for

→ Interpolation (You have already seen)
→ Differentiation (This also you saw)
→ Integration (Will see now).

As the integration will be done by the numerical methods based on polynomial approximations such integrations are also called quadratures.



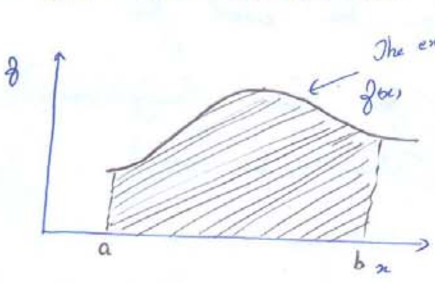
→ From the given data set if you want to evaluate $I = \int_a^b f(x)\,dx$

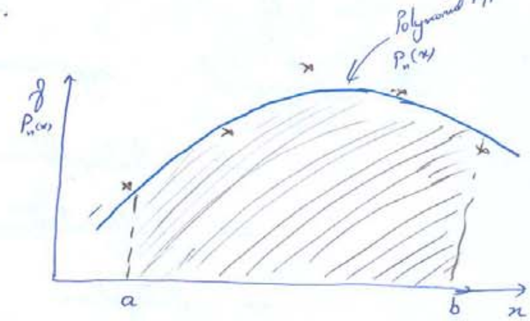
Then as $f(x) \approx P_n(x)$

$$I \approx \int_a^b P_n(x)\,dx$$

Q: Whether the integration you do by such method is exact (without error)?!

Your polynomial $P_n(x)$ is only approximating $f(x)$. ∴ The integration will also be not that accurate.





⇒ You have studied

* Direct-fit polynomials
* Lagrange polynomials
* Newton's forward and backward difference polynomials, etc.

⇒ You can utilise these polynomials to evaluate integration between any data points.

<u>Direct-Fit</u>

If you have a direct-fit polynomial

$$P_n(x) = a_0 + a_1 x + a_2 x^2 + \dots + a_n x^n$$

for a given set of data, then

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

$$= \int_a^b (a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n)\,dx$$

→ You may require some computational time to evaluate $a_0, a_1, a_2, \ldots a_n$.

Newton - Cotes Formulas

For equally spaced data, you can use Newton's forward difference polynomial for approximating the function. If such polynomials are used for integration, then the resulting integration formulas are called Newton - Cotes Formulas.

i.e. $$I = \int_a^b f(x)\,dx \cong \int_a^b P_n(x)\,dx$$

where $$P_n(x) = f_0 + s\,\Delta f_0 + \frac{s(s-1)}{2}\Delta^2 f_0 + \frac{s(s-1)(s-2)}{3!}\Delta^3 f_0 + \cdots + \frac{s(s-1)(s-2)\cdots(s-(n-1))}{n!} + \text{Error}$$

where $$s = \frac{x - x_0}{\Delta x}$$

$$\text{Error} = \frac{s(s-1)(s-2)\cdots(s-n)}{(n+1)!}\Delta h^{n+1} f^{(n+1)}(\xi)$$

$$x_0 \le \xi \le x_n$$

$$\therefore \quad I = \int_a^b f(x)\,dx \cong \int_a^b P_n(x)\,dx$$

$$= \Delta x \int_{s_a}^{s_b} P_n(s)\,ds \qquad \left(\because\ ds = \frac{dx}{\Delta x}\right)$$

$$s_a = \frac{a - x_0}{\Delta x} \quad \text{and} \quad s_b = \frac{b - x_0}{\Delta x}$$

⇒ Now if the lower limit $x = a$ of the integration is fixed as base point in developing $P_n(x)$,

i.e. $x_0 = a$

$\therefore$ At $x = a$, $\quad s = 0$

and at $x = b$, $\quad s = \dfrac{b-a}{\Delta x}$

$$\therefore \quad I = \Delta x \int_{s_a}^{s_b} P_n(s)\,ds$$

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

You know $P_n(x)$ and $P_n(s)$ are same and $x = x_0 + s\Delta x$

$$\therefore \quad I = \Delta x \int_0^s P_n(x_0 + s\Delta x)\,ds$$

Based on the degree of polynomial $P_n(x_0 + s\Delta x)$, we will get different types of Newton-Cotes formulas.

i) When $n = 0$:

$$I = \Delta x \int_0^s P_0(x_0 + s\Delta x)\,ds = \Delta x \int_0^s c\,ds = \underline{\underline{c\,s\,\Delta x}}$$

This is Rectangular Formula.

ii) When $n = 1$:

$$I = \Delta x \int_0^s P_1(x_0 + s\Delta x)\, ds$$

$$= \Delta x \int_0^s \left[f_0 + s\,\Delta f_0 \right] ds = \Delta x \left[s f_0 + \frac{s^2}{2} \Delta f_0 \right]$$

~~i.e. I =~~

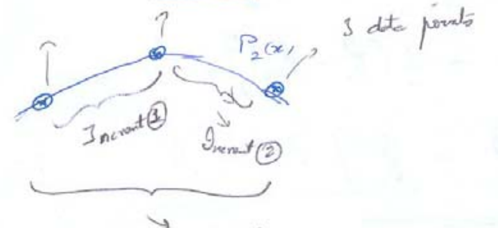
Note: ⇒ Range of integration (distance b/w lower and upper limits of integration)

Increment (distance b/w any two data points)

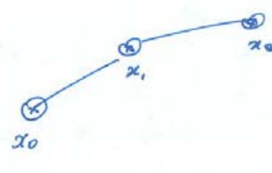
∴ A linear polynomial requires one increment and two data points to fit.

Second degree polynomial requires two increments and three data points to fit.

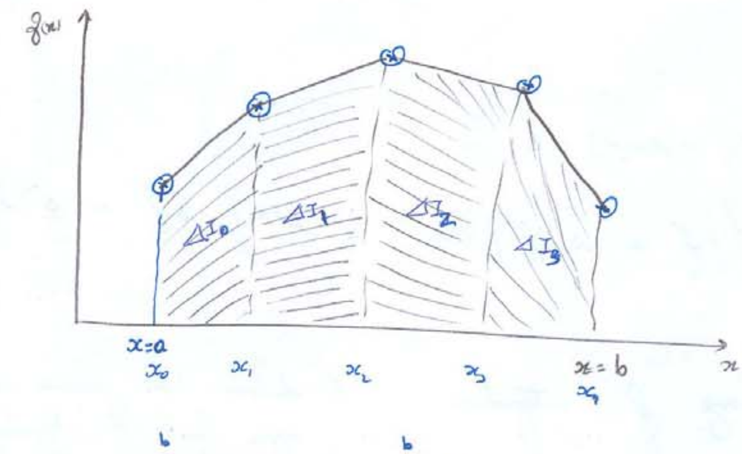
A group of increments required to fit a polynomial is called interval.



One Interval for $P_2(x)$ having two increments.



That way when $n = 1$, linear polynomial is fit.



$$I = \int_a^b f(x)\,dx = \int_a^b P_1(x)\,dx$$

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

Now $I = \Delta I_0 + \Delta I_1 + \Delta I_2 + \Delta I_3$

~~$\Delta I_1 = \Delta x \int_0$~~ At $x = x_1$, $s = 1.0$

$$\therefore \Delta I_0 = \Delta x \int_0^1 \left[f_0 + s\Delta f_0\right] ds$$

$$= \Delta x \left[f_0 + \tfrac{1}{2}\Delta f_0\right]$$

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

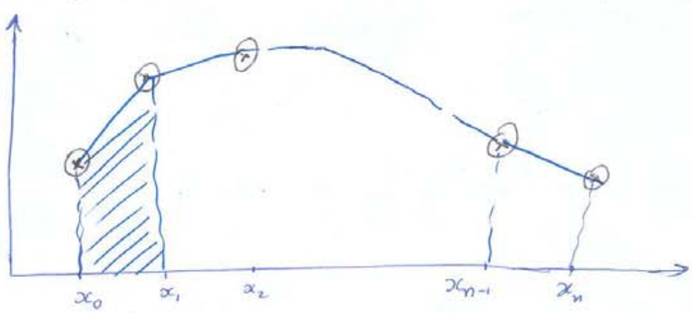
$$\Delta I_0 = \frac{\Delta x}{2}\left[f_0 + f_1\right]$$

In the same way $\int_{x_1}^{x_2} P_1(x)\,dx = \frac{\Delta x}{2}\left[f_1 + f_2\right]$

This is the famous Trapezoidal Rule to find the area or integration.

If we actually want to find the integration from $x = a$ to $x = b$ then we need to add all those ΔI's to obtain composite trapezoidal rule.

$\Rightarrow$ So if we want to find integrate from $x = x_0$ to $x = x_n$, there are $(n+1)$ data points.



Then 'n' $\rightarrow$ elements are there

$$I = \Delta I_0 + \Delta I_1 + \Delta I_2 + \cdots\cdots + \Delta I_{n-1}$$

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

For equally spaced data:

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

$\Rightarrow$ For a single interval

$$E_{rr} = \Delta x \int_0^1 \frac{s(s-1)}{2} \Delta x^2 f''(\xi)\, ds = -\frac{1}{12} \Delta x^3 f''(\xi)$$

$\hookrightarrow O(\Delta x^3)$

However, total error in (global) $= \sum_{i=0}^{n-1} (E_{rr}) = \sum_{i=0}^{n-1} \left[\frac{-1}{12} \Delta x^3 f''(\xi) \right]$

$$= -\frac{n}{12} \Delta x^3 f''(\xi) = \frac{x_n - x_0}{\Delta x} \Delta x^3 f''(\xi) \rightarrow O(\Delta x^2)$$