Lecture-10
Algorithmic Mathematics(CSC545)

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Numerical differentiation

- **Numerical differentiation** is the process of finding the **numerical** value of a **derivative** of a given function at a given point.

11.2 DIFFERENTIATING CONTINUOUS FUNCTIONS

We discuss here the numerical process of approximating the derivative $f'(x)$ of a function $f(x)$, when the function itself is available.

Forward Difference Quotient

Consider a small increment $\Delta x = h$ in x. According to Taylor's theorem, we have

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\theta) \tag{11.1}$$

for $x \le \theta \le x + h$. By rearranging the terms, we get

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(\theta) \tag{11.2}$$

Thus, if h is chosen to be sufficiently small, $f'(x)$ can be approximated by

$$\boxed{f'(x) = \frac{f(x+h) - f(x)}{h}} \tag{11.3}$$

with a truncation error of

$$\boxed{E_t(h) = -\frac{h}{2} f''(\theta)} \tag{11.4}$$

Equation (11.3) is called the first order *forward difference quotient*. This is also known as *two-point formula*. The truncation error is in the order of h and can be decreased by decreasing h.

Similarly, we can show that the first-order *backward difference quotient* is

$$\boxed{f'(x) = \frac{f(x) - f(x-h)}{h}} \tag{11.5}$$

Estimate approximate derivative of $f(x) = x^2$ at $x = 1$, for $h = 0.2, 0.1, 0.05$ and 0.01 using the first-order forward difference formula.

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

Therefore,

$$f'(1) = \frac{f(1+h) - f(1)}{h}$$

Derivative approximations are tabulated below:

h	$f'(1)$	*Error*
0.2	2.2	0.2
0.1	2.1	0.1
0.05	2.05	0.05
0.01	2.01	0.01

Central Difference Quotient

Note that Eq. (11.3) was obtained using the linear approximation to $f(x)$. This would give large truncation errors if the functions were of higher order. In such cases, we can reduce truncation errors for a given h by using a quadratic approximation, rather than a linear one. This can be achieved by taking another term in Taylor's expansion, i.e.,

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(\theta_1) \qquad (11.6)$$

Similarly,

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(\theta_1) \tag{11.7}$$

Subtracting Eq. (11.7) from Eq. (11.6), we obtain

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3!} [f'''(\theta_1) + f'''(\theta_2)] \tag{11.8}$$

Thus, we have

$$\boxed{f'(x) = \frac{f(x+h) - f(x-h)}{2h}} \tag{11.9}$$

with the truncation error of

$$E_t(h) = -\frac{h^2}{12} [f'''(\theta_1) + f'''(\theta_2)] = -\frac{h^2}{6} f'''(\theta)$$

which is of order h^2. Equation (11.9) is called the second-order *central difference quotient*. Note that this is the average of the forward difference quotient and the backward difference quotient. This is also known as *three-point formula*. The distinction between the two-point and three-point formulae is illustrated in Fig. 11.1(a) and Fig. 11.1(b). Note that the approximation is better in the case of three-point formula.

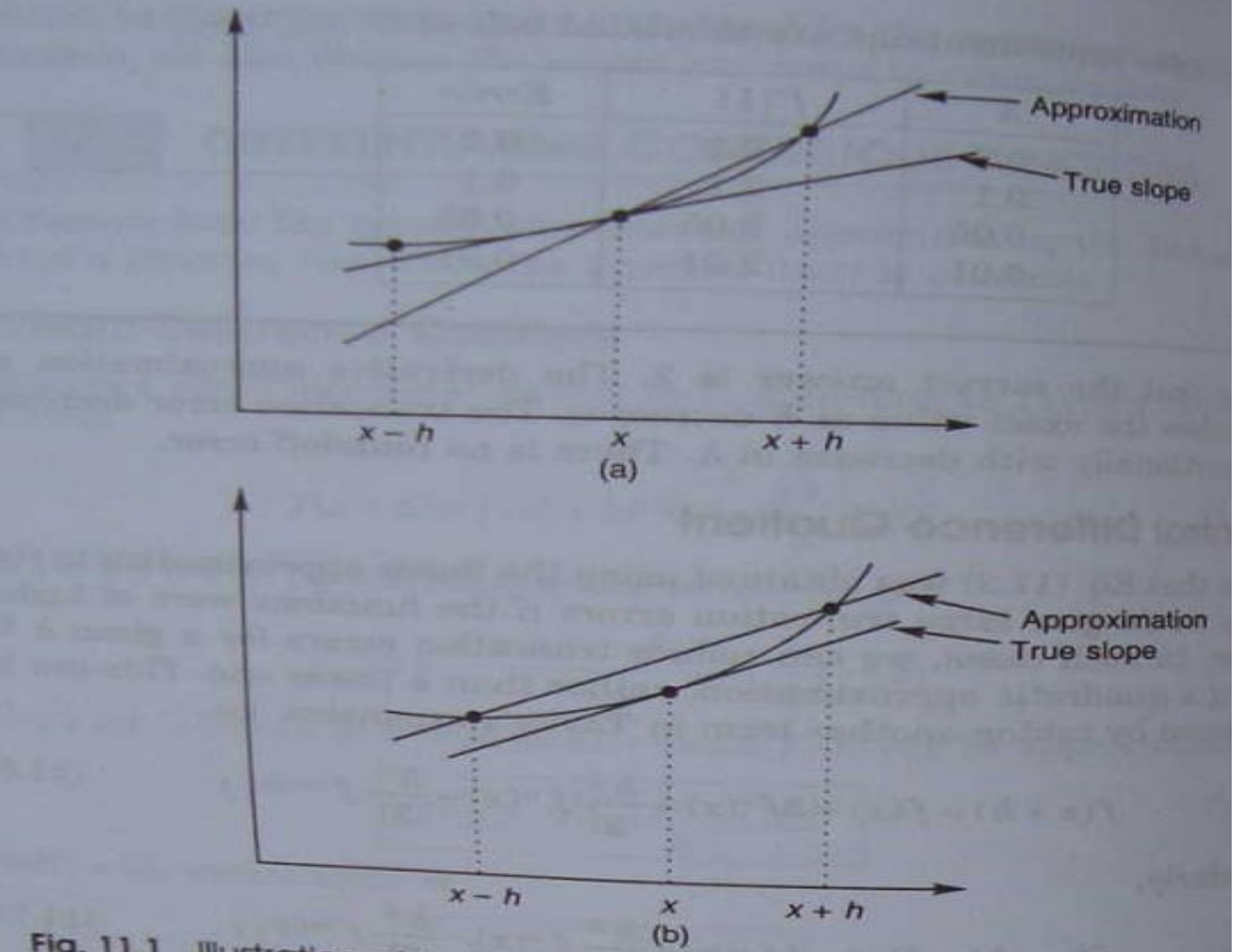

Fig. 11.1 Illustration of (a) Two-point formula and (b) Three-point formu

Numerical Integration

- **Numerical integration** is the approximate computation of an **integral** using **numerical** techniques. The **numerical** computation of an **integral** is sometimes called quadrature

case with experimental data.

We know that a definite integral of the form

$$I = \int_a^b f(x)\,dx \qquad (12.1)$$

can be treated as the area under the curve $y = f(x)$, enclosed between the limits $x = a$ and $x = b$. This is graphically illustrated in Fig. 12.1. The problem of integration is then simply reduced to the problem of finding the shaded area.

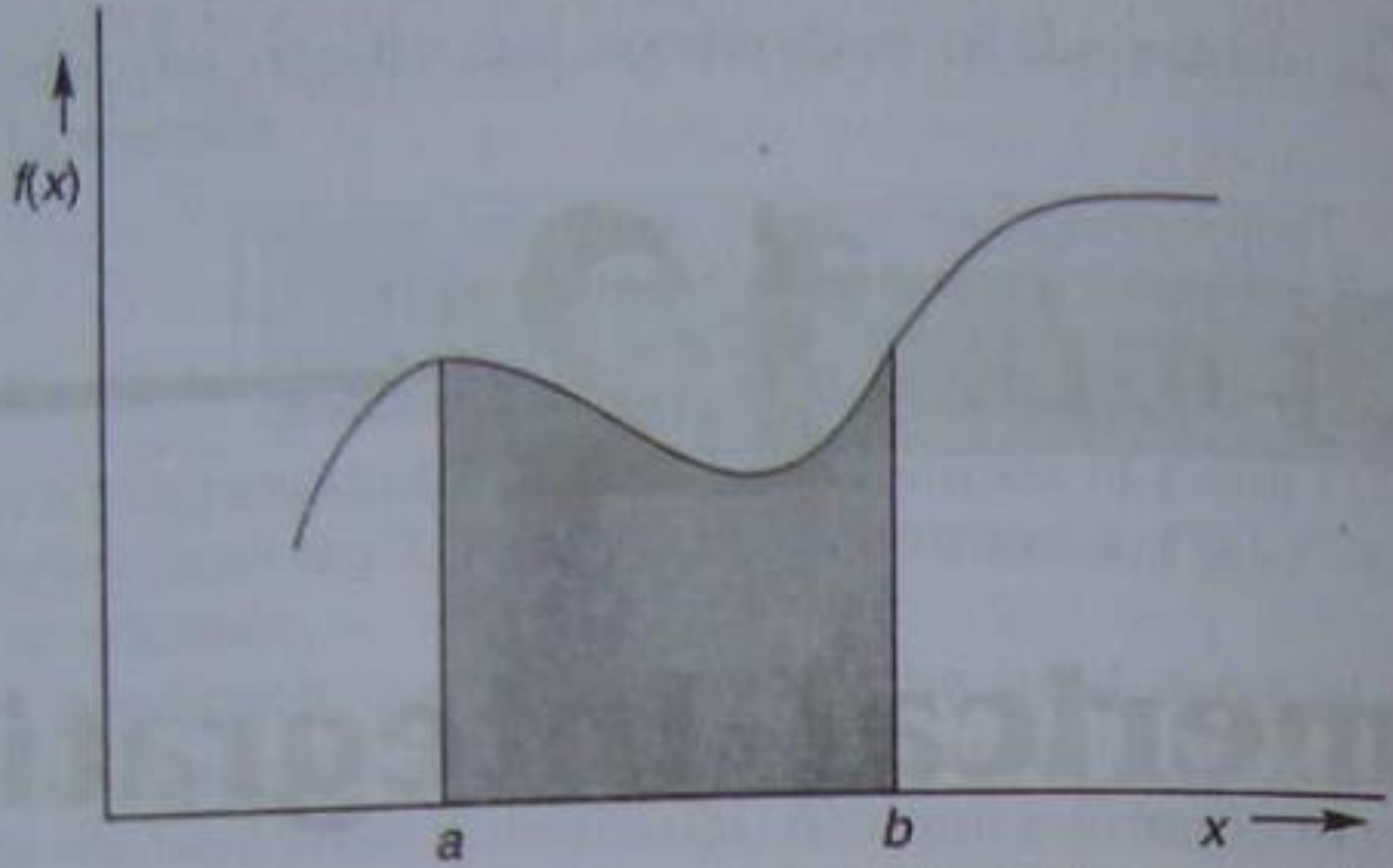

Fig. 12.1 Graphical representation of integral of a function

$$I = \int_a f(x)\,dx = \int_a p_n(x)\,dx$$

We know that the polynomial $p_n(x)$ can be easily integrated analytically. Equation (12.2) can be expressed in summation form as follows:

$$\int_a^b p_n(x)\,dx = \sum_{i=0}^{n} w_i\, p_n(x_i) \tag{12.3}$$

where $a = x_0 < x_1 < \ldots < x_n = b$

Since $p_n(x)$ coincides with $f(x)$ at all the points x_i, $i = 0, 1, \ldots n$, we can say that,

$$\boxed{I = \int_a^b f(x)\,dx \approx \sum_{i=0}^{n} w_i\,(x_i)} \tag{12.4}$$

The values x_i are called *sampling points* or *integration nodes* and the constants w_i are called *weighting coefficients* or simply *weights*.

Equation (12.4) provides the basic integration formula that will be extensively used in this chapter. Note that the interpolation polynomial

12.2 NEWTON-COTES METHODS

Newton-Cotes formula is the most popular and widely used numerical integration formula. It forms the basis for a number of numerical integration methods known as *Newton-Cotes methods*.

The derivation of Newton-Cotes formula is based on polynomial interpolation. As pointed our earlier, an nth degree polynomial $p_n(x)$ that interpolates the values of $f(x)$ at $n + 1$ evenly spaced points can be used to replace the integrand $f(x)$ of the integral

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

and the resultant formula is called $(n + 1)$ point *Newton-Cotes formula*. If the limits of integration a and b are in the set of interpolating points x_i, $i = 0, 1, \ldots n$, then the formula is referred to as *closed form*. If the points a and b lie beyond the set of interpolating points, then the formula is termed *open form*. Since open form formula is not used for definite integration, we consider here only the closed form methods. They include:

1. Trapezoidal rule (two-point formula)
2. Simpson's 1/3 rule (three-point formula)
3. Simpson's 3/8 rule (four-point formula)
4. Boole's rule (five-point formula)

All these rules can be formulated using either Newton or Lagrange interpolation polynomial for approximating the function $f(x)$. We use here the Newton-Gregory forward formula (Eq. (9.20)) which is given below:

$$p_n(s) = f_0 + \Delta f_0 s + \frac{\Delta^2 f_0}{2!} s(s-1) + \frac{\Delta^3 f_0}{3!} s(s-1)(s-2) + \ldots$$

$$= T_0 + T_1 + T_2 + \ldots + T_n \tag{12.5}$$

where

$$s = (x - x_0)/h$$

and

$$h = x_{i+1} - x_i$$

12.3 TRAPEZOIDAL RULE

The trapezoidal rule is the first and the simplest of the Newton-Cotes formulae. Since it is a two-point formula, it uses the first order interpolation polynomial $p_1(x)$ for approximating the function $f(x)$ and assumes $x_0 = a$ and $x_1 = b$. This is illustrated in Fig. 12.2. According to Eq. (12.5), $p_1(x)$ consists of the first two terms T_0 and T_1. Therefore, the integral for trapezoidal rule is given by

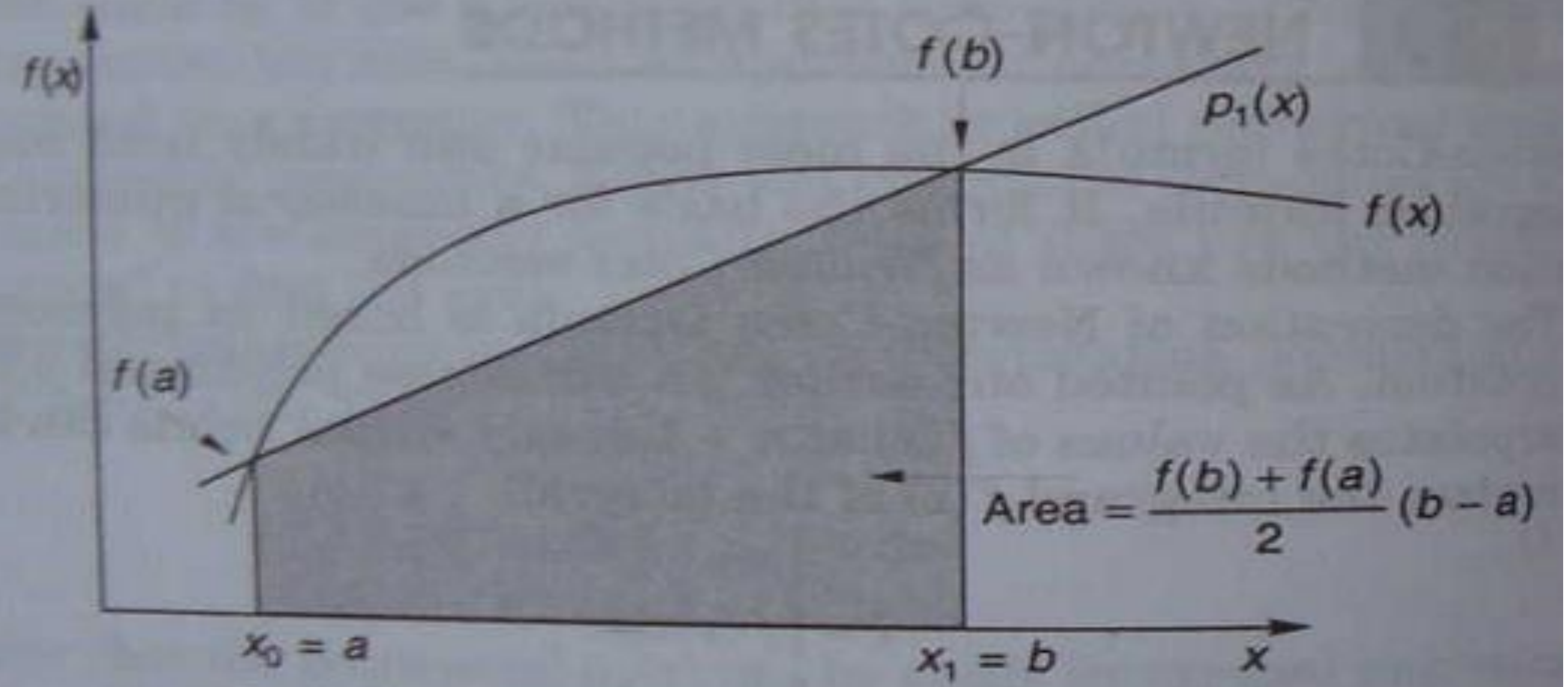

Fig. 12.2 Representation of trapezoidal rule

$$I_t = \int_a^b (T_0 + T_1)\,dx$$

$$= \int_a^b T_0\,dx + \int_a^b T_1\,dx = I_{t1} + I_{t2}$$

Since T_i are expressed in terms of s, we need to use the following transformation:

$$dx = h \times ds$$

$$x_0 = a, \quad x_1 = b \quad \text{and} \quad h = b - a$$

At $\quad x = a, \quad s = (a - x_0)/h = 0$

At $\quad x = b, \quad s = (b - x_0)/h = 1$

Then,

$$I_{t1} = \int_a^b T_0 \; dx = \int_0^1 hf_0 \; dx = hf_0$$

$$I_{t2} = \int_a^b T_1 \; dx = \int_0^1 \Delta f_0 \; sh \; ds = h\frac{\Delta f_0}{2}$$

Therefore,

$$I_t = h\left[f_0 + \frac{\Delta f_0}{2}\right] = h\left[\frac{f_0 + f_1}{2}\right]$$

Since $f_0 = f(a)$ and $f_1 = f(b)$, we have

$$\boxed{I_t = h\,\frac{f(a) + f(b)}{2} = (b - a)\,\frac{f(a) + f(b)}{2}} \qquad (12.6)$$

Note that the area is the *product of width of the segment* $(b - a)$ *and average height of the points* $f(a)$ *and* $f(b)$.

Error Analysis

Since only the first two terms of eq. (12.5) are used for I_t, the term T_2 becomes the remainder and, therefore, the truncation error in trapezoidal rule is given by

$$E_{tt} = \int_a^b T_2 \, dx = \frac{f''(\theta_s)}{2} \int_0^1 s(s-1)h \cdot ds$$

$$= \frac{f''(\theta_s)h}{2}\left[\frac{s^3}{3} - \frac{s^2}{2}\right]_0^1 = -\frac{f''(\theta_s)}{12}h$$

Since $dx/ds = h$,

$$f''(\theta_s) = h^2 f''(\theta_x),$$

we obtain

$$\boxed{E_{tt} = -\frac{h^3}{12} f''(\theta_x)} \qquad (12.7)$$

where $a < \theta_x < b$

Evaluate the integral

$$I = \int_a^b (x^3 + 1)\,dx$$

for the intervals (a) (1, 2) and (b) (1, 1.5)
Also estimate truncation error in each case and compare the results with the exact answer.

Case a $\quad a = 1, b = 2$

$h = 1$

$$I_t = \frac{b-a}{2}\,[f(a) + f(b)]$$

$$= \frac{1}{2}\,(2 + 9) = 5.5$$

$$|E_{tt}| \le \frac{h^3}{12} \max_{1 \le x \le 2} |f''(x)|$$

$$f''(x) = 6x$$

$$\max_{1 \le x \le 2} |f''(x)| = f''(2) = 12$$

Therefore,

$$|E_{tt}| \le \frac{h^3}{12}\, f''(2) = 1$$

$$I_{\text{exact}} = 9.75$$

$$\text{True error } = I_t - I_{\text{exact}} = 0.75$$

$I_{exact} = 0.75$

Note that the error bound is an overestimate of the true error.

Case b

$$a = 1, b = 1.5$$

$$h = 0.5$$

$$I_t = \frac{0.5}{2}[f(1) + f(1.5)] = 1.59375$$

$$|E_{tt}| = \frac{(0.5)^3}{12} f''(1.5) = 0.09375$$

$$I_{exact} = 1.515625$$

$$\text{True error} = 0.078125$$

Composite Trapezoidal Rule

If the range to be integrated is large, the trapezoidal rule can be improved by dividing the interval (a, b) into a number of small intervals and applying the rule discussed above to each of these subintervals. The sum of areas of all the subintervals is the integral of the interval (a, b). This is known as *composite* or *multisegment approach*. This is illustrated in Fig. 12.3.

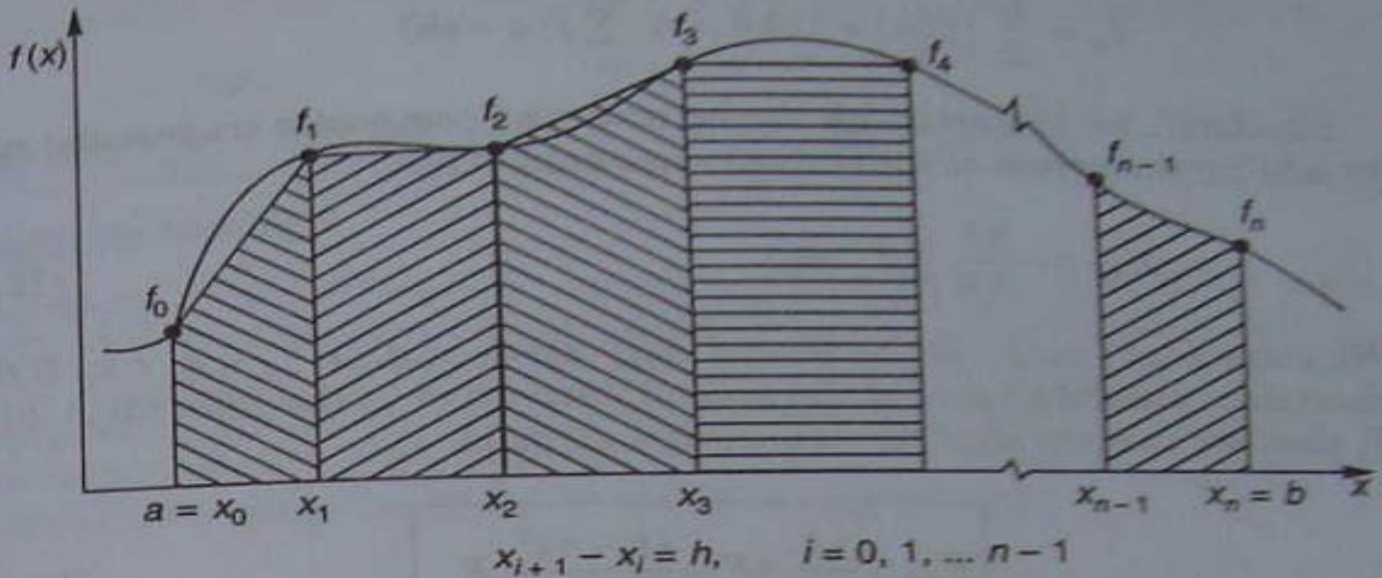

Fig. 12.3 Multisegment trapezoidal rule

As seen in Fig. 12.3, there are $n + 1$ equally spaced sampling points that create n segments of equal width h given by

$$h = \frac{b-a}{n}$$

$$x_i = a + ih, \qquad i = 0, 1, \dots, n$$

From Eq. (12.6), area of the subinterval with the nodes x_{i-1} and x_i, is given by

$$I_i = \int_{x_{i-1}}^{x_i} p_1(x)\, dx = \frac{h}{2}\,[f(x_{i-1}) + (x_i)]$$

The total area of all the n segments is

$$I_{ct} = \sum_{i=1}^{n} \frac{h}{2} [f(x_{i-1}) + f(x_i)]$$

$$= \frac{h}{2} [f(x_0) + f(x_1)] + \frac{h}{2} [f(x_1) + f(x_2)]$$

$$+ \ldots + \frac{h}{2} [f(x_{n-1}) + f(x_n)]$$

Denoting $f_i = f(x_i)$ and regrouping the terms, we get

$$\boxed{I_{ct} = \frac{h}{2}\left[f_0 + 2\sum_{i=1}^{n-1} f_i + f_n \right]} \tag{12.8}$$

Equation (12.8) is the general form of trapezoidal rule and is known as *composite trapezoidal rule*. Equation (12.8) can also be expressed as follows:

Compute the integral

$$\int_{-1}^{1} e^{x}\, dx$$

using composite trapezoidal rule for (a) $n = 2$ and (b) $n = 4$.

Case a

$$n = 2$$

$$h = \frac{b-a}{2} = \frac{2}{2} = 1$$

$$I_{ct} = \frac{h}{2}\,[f(a) + f(b)] + h\sum_{i=1}^{n-1} f(a + ih)$$

$$= \frac{1}{2}\,[\exp(-1) + \exp(1)] + \exp(0)$$

$$= 2.54308$$

Case b

$$n = 4$$

$$h = \frac{b-a}{4} = 0.5$$

$$= \frac{0.5}{2} + [\exp(-1) + \exp(1)] + [\exp(-0.5) + \exp(0) + \exp(0.5)]\ 0.5$$

$$= 2.39917$$

Note that $I_{exact} = 2.35040$ and $n = 4$ gives better results.

Assignment#10

Use the trapezoidal rule with $n = 4$ to estimate

$$\int_0^1 \frac{dx}{1+x^2}$$

correct to five decimal places.

Thank You

Any Query??