Chapter 6

Numerical Differentiation and Integration

Numerical Differential Techniques

- Use the forward, backward and central difference formula to approximate the first derivative of the function $f(x) = 2e^{1.5x}$ at $x = 3$ taking h = 0.1.
- or, Estimate the first derivative $f'(x)$ at x = 3 using numerical techniques with step size h = 0.1 for the function $f(x)$ = $2e^{1.5x}$

Here,

$f(x) = 2e^{1.5x}$

a = 3

h = 0.1

1. **Forward difference:**

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

$$= \frac{f(3+0.1)-f(3)}{0.1}$$

$$= \frac{f(3.1)-f(3)}{0.1}$$

$$= \frac{2e^{1.5(3.1)} - 2e^{1.5(3)}}{0.1}$$

= 291.357

2. **Backward difference:**

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

$$= \frac{f(3)-f(3-0.1)}{0.1}$$

$$= \frac{f(3)-f(2.9)}{0.1}$$

$$= \frac{2e^{1.5(3)} - 2e^{1.5(2.9)}}{0.1}$$

= 250.773

3. **Central difference:**

$$\boldsymbol{f'(x) = \frac{f(a+h)-f(a-h)}{2h}}$$

$$= \frac{f(3+0.1)-f(3-0.1)}{2(0.1)}$$

$= \frac{f(3.1) - f(2.9)}{0.2}$

$= \frac{2e^{1.5(3.1)} - 2e^{1.5(2.9)}}{0.2}$

= 271.065

Error:

$$\text{Relative Error} = \left| \frac{\text{Exact} - \text{Approximate}}{\text{Exact}} \right| \times 100\%$$

Exact value at x = 3:

$f(x) = 2e^{1.5x}$

$\boldsymbol{f'(x)} = 3e^{1.5x}$

$= 3e^{1.5(3)}$

= 270.051

Numerical Integration:

Newton-Cotes Integration Methods

Newton-Cotes methods are a group of techniques used to estimate the area under a curve, also known as numerical integration.

Sometimes, the function that we want to integrate (find the area under) is too complicated, or maybe we only have a table of data points instead of an actual formula. In these cases, we use Newton-Cotes methods.

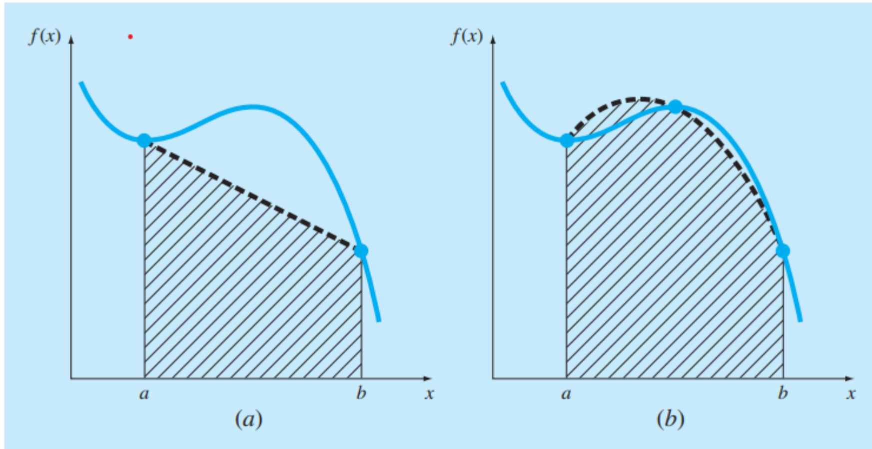
- Newton-Cotes methods are the most common numerical integration schemes.
- Replace the complicated function f(x) with a simpler function called f_n(x).
- This simpler function f_n(x) is a polynomial that approximates the original function.

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

Where $f_n(x)$ is a polynomial of the form

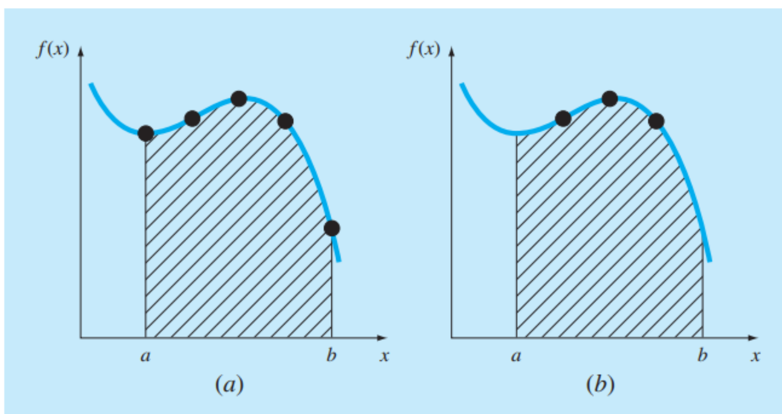
$$f_n(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

FIGURE 21.1
The approximation of an integral by the area under (*a*) a single straight line and (*b*) a single parabola.



Closed and open forms of the Newton-Cotes formulas are available. The closed forms are those where the data points at the beginning and end of the limits of integration are known (Fig. 21.3a). The open forms have integration limits that extend beyond the range of the data (Fig. 21.3b). In this sense, they are akin to extrapolation.

FIGURE 21.3
The difference between (*a*) closed and (*b*) open integration formulas.



1st Order Method (Trapezoidal Rule):

The trapezoidal rule is the first of the Newton-Cotes closed integration formulas. It corresponds to the case where the polynomial used is a first order:

$$I = \int_a^b f(x)dx \cong \int_a^b f_1(x)dx$$

A straight line can be represented as

$$f_1(x) = f(a) + \frac{f(b) - f(a)}{b - a}(x - a)$$

The area under this straight line is an estimate of the integral of $f(x)$ between the limits a and b:

$$I = \int_a^b \left[f(a) + \frac{f(b) - f(a)}{b - a}(x - a)\right] dx$$

Now, we split it into two terms:

$$I = \int_a^b f(a)\, dx + \int_a^b \frac{f(b) - f(a)}{b - a}(x - a) dx$$

Here, by integrating the first and second part we get,

$$\int_a^b f(a)\, dx = \ f(a).(b - a)$$

Since, $f(a)$ is a constant.

$$\int_a^b \frac{f(b) - f(a)}{b - a}(x - a) dx$$
$$= \frac{f(b)-f(a)}{b-a} \int_a^b (x - a) dx$$
$$= \frac{f(b)-f(a)}{b-a} \left[\frac{(x-a)^2}{b-a} \right]_a^b$$
$$= \frac{f(b)-f(a)}{b-a} \frac{(b-a)^2}{2}$$
$$= \frac{f(b)-f(a)}{2}(b - a)$$

By adding both parts we get,

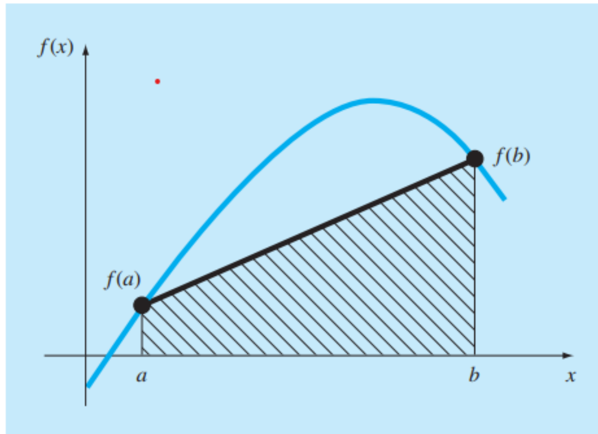
$$I = f(a).(b - a) + \frac{f(b) - f(a)}{2}(b - a)$$

$$I = (b - a) \left[f(a) + \frac{f(b) - f(a)}{2}\right]$$

$$I = (b - a)\frac{f(a) + f(b)}{2}$$

And this is the expression for the trapezoidal method.

FIGURE 21.4
Graphical depiction of the trapezoidal rule.

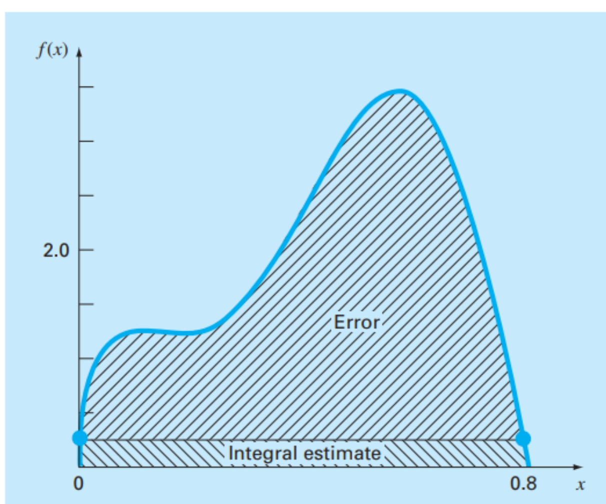


When we employ the integral under a straight-line segment to approximate the integral under a curve, we obviously can incur an error that may be substantial (Fig. 21.6). An estimate for the local truncation error of a single application of the trapezoidal method is

$$E = \mathcal{O}((b-a)^3)$$

Definition of E indicates that if the function being integrated is linear, the trapezoidal rule will be exact. Otherwise, for functions with second- and higher-order derivatives (that is, with curvature), some error can occur.

FIGURE 21.6
Graphical depiction of the use of a single application of the trapezoidal rule to approximate the integral of $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ from $x = 0$ to 0.8.



Multiple Applications of Trapezoidal Method

One way to improve the accuracy of the trapezoidal rule is to divide the integration interval from a to b into a number of segments and apply the method to each segment (Fig. 21.7). The areas of individual segments can then be added to yield the integral for the entire interval.

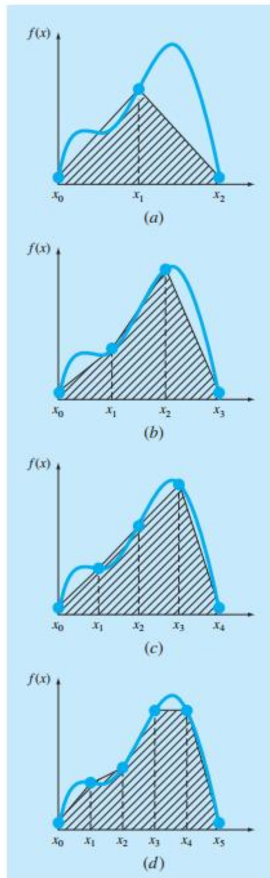


FIGURE 21.7
Illustration of the multiple-application trapezoidal rule. (a) Two segments, (b) three segments, (c) four segments, and (d) five segments.

Figure 21.8 shows the general format and nomenclature we will use to characterize multiple-application integrals. There are n+1 equally spaced points $x_0, x_1, \dots x_n$. Consequently, there are n segments of equal width of h:

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

If we set $a = x_0$ and $b = x_n$ then the total integral is

$$I = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)dx$$

Substituting the trapezoidal method for each integral, yields

$$I = h\frac{f(x_0) + f(x_1)}{2} + h\frac{f(x_1) + f(x_2)}{2} + \cdots + h\frac{f(x_{n-1}) + f(x_n)}{2}$$

$$I = \frac{h}{2}[f_0 + 2(f_1 + f_2 + f_3 + \cdots + f_{n-1}) + f_n]$$

$$I = \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right]$$

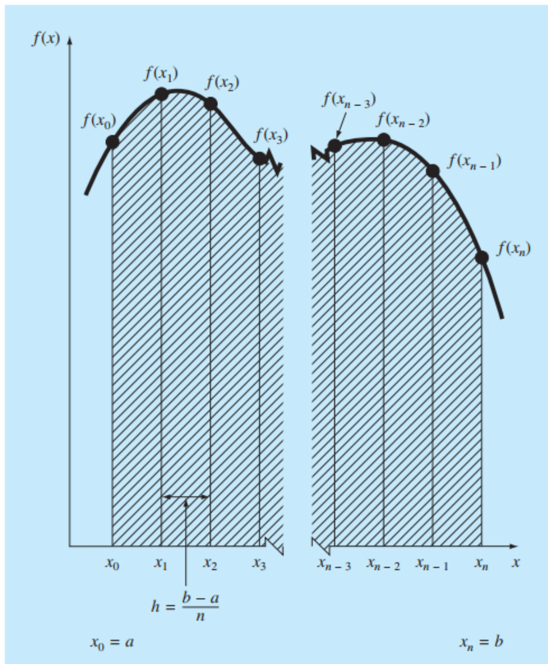


FIGURE 21.8
The general format and nomenclature for multiple-application integrals.

For the case of multiple application of the Trapezoidal method the approximation error becomes

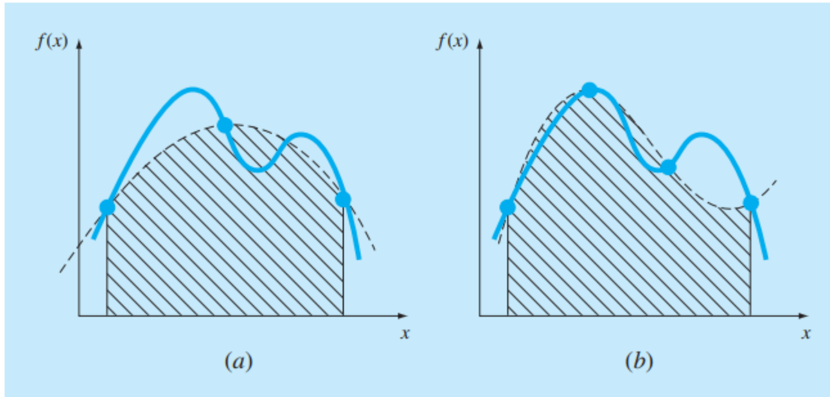
$$E = \mathcal{O}\left(\frac{(b-a)^3}{n^2}\right)$$

Math example: S.S Sastry (Example 6.8)

2nd Order Method (Simpon's Rule):

Aside from applying the trapezoidal rule with finer segmentation, another way to obtain a more accurate estimate of an integral is to use higher-order polynomials to connect the points. For example, if there is an extra point midway between f(a) and f(b), the three points can be connected with a parabola (Fig. 21.10a). If there are two points equally spaced between f(a) and f(b), the four points can be connected with a third-order polynomial (Fig. 21.10b).

FIGURE 21.10
(a) Graphical depiction of Simpson's 1/3 rule: It consists of taking the area under a parabola connecting three points. (b) Graphical depiction of Simpson's 3/8 rule: It consists of taking the area under a cubic equation connecting four points.



This method can be derived as following

$$I = \int_a^b f(x)dx \cong \int_a^b f_2(x)dx$$

If we let $a = x_0$ and $b = x_2$ and $f_2(x)$ is represented by a second order Lagrange polynomial, the integral becomes

$$I = \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2)\right] dx$$

After integration and some algebraic manipulation, the following expressions arises,

$$I \cong \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)]$$

Where for this case, $h \stackrel{\text{def}}{=} (b-a)/2$. The error can be computed as

$$E = \mathcal{O}((b-a)^5)$$

Multiple Application of the 2nd Order Method

We can also apply this method on multiple segments of equally divided interval with $h = \frac{b-a}{n}$
The total integral can be expressed as

$$I = \int_{x_0}^{x_2} f_2(x)dx + \int_{x_2}^{x_4} f_2(x)dx + \cdots + \int_{x_{n-2}}^{x_n} f_2(x)dx$$

Substituting the Simpson's 1/3 rule for each integral, yields

$$I \cong 2h\frac{f(x_0) + 4f(x_1) + f(x_2)}{6} + \cdots + 2h\frac{f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)}{6}$$

$$I \cong \frac{h}{3}\left[f(x_0) + 4\sum_{i=1,odd\ i}^{n-1} f(x_i) + 2\sum_{j=2,even\ j}^{n-2} f(x_j) + f(x_n)\right]$$

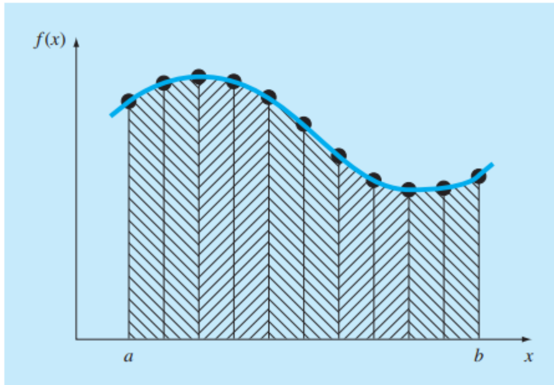


FIGURE 21.11
Graphical representation of the multiple application of Simpson's 1/3 rule. Note that the method can be employed only if the number of segments is even.

The error estimate is

$$E = \mathcal{O}\left(\frac{(b-a)^5}{n^4}\right)$$

Simpon's 3/8 rule:

- Fits a third-degree (cubic) polynomial through 4 points
- Uses 3 subintervals at a time
- Number of intervals is must be divisible by 3

$$I \cong \frac{3h}{8}[y_0 + 3(y_1 + y_2 + y_4 + \cdots + y_{n-1}) + 2(y_3 + y_6 + y_9 + \ldots + y_{n-3}) + y_n]$$

Example:

Find the area under the curve from $\int_0^3 \frac{1}{1+x^2}\, dx$ using i) Trapezoidal Rule, ii) Simpson's 1/3 Rule, iii) Simpson's 3/8 Rule. Compare the error for each of the method.

Solution:

We get,

$$\int_0^3 \frac{1}{1+x^2}\, dx = [\tan^{-1} x]_0^3 = \tan^{-1}(3) - \tan^{-1}(0)$$

$$= \tan^{-1}(3) = 1.2490\ (approx)$$

Let, number of intervals, n = 6

So, step size, h = $\frac{3-0}{6}$ = 0.5

x	$f(x) = \frac{1}{1+x^2}$
0.0	1.0000
0.5	0.8000
1.0	0.5000
1.5	0.3077
2.0	0.2000
2.5	0.1379
3.0	0.1000

Trapezoidal Method:

$$I = \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right]$$

$$I = \frac{h}{2}[f_0 + 2(f_1 + f_2 + f_3 + \cdots + f_{n-1}) + f_n]$$

$$= \frac{0.5}{2}[1 + 2(0.8 + 0.5 + 0.3077 + 0.2 + 0.1379) + 0.1]$$

= 0.25(4.9912)

= 1.2478 (approx.)

Simpon's 1/3 Rule (Even number of intervals, n= 6):

$$I \cong \frac{h}{3}[f_0 + 4(f_1 + f_3 + f_5) + 2(f_2 + f_4) + f_6]$$

$= \frac{0.5}{3}[1 + 4(0.8 + 0.3077 + 0.1379) + 2(0.5 + 0.2) + 0.1]$

$= \frac{0.5}{3}(7.4824)$

= 1.2475 (approx.)

Simpson's 3/8 Rule (number of intervals divisible by 3, n = 6):

$$I \cong \frac{3h}{8}[f_0 + 3(f_1 + f_2 + f_4 + f_5) + 2(f_3) + f_6]$$

$= \frac{3(0.5)}{8}(1 + 3(0.8 + 0.5 + 0.2 + 0.1379) + 2(0.3077) + 0.1]$

$= \frac{3(0.5)}{8}(7.4824)$

= 1.2417(approx.)

Example: S.S.Sastry (6.9, 6.10)