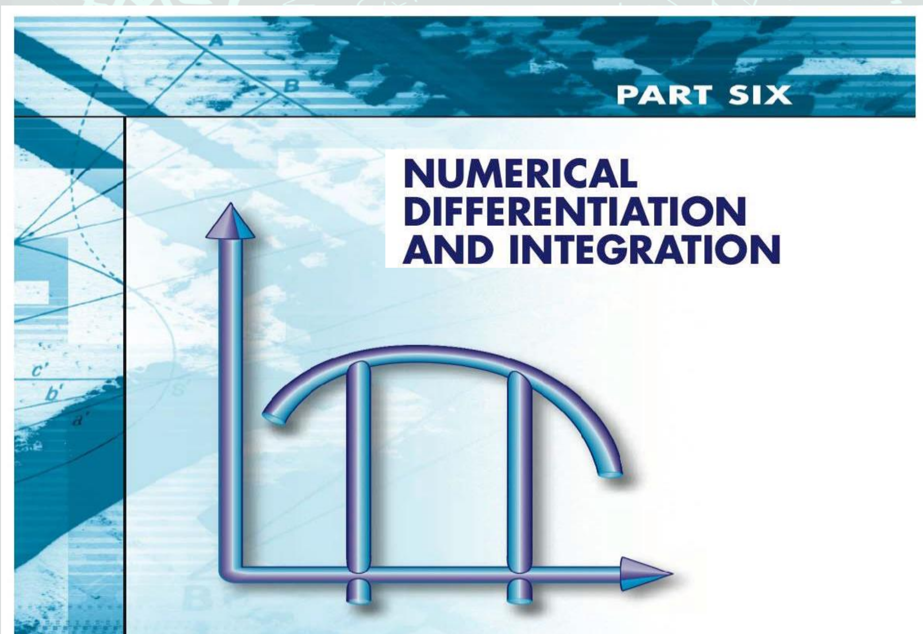
ریاضیات عالی پیشرفته

Numerical Methods for Engineers

مدرس دکتر پدرام پیوندی



Newton-Cotes Integration Formulas

The *Newton-Cotes formulas* are the most common numerical integration schemes. They are based on the strategy of replacing a complicated function or tabulated data with an approximating function that is easy to integrate:

$$I = \int_a^b f(x)\,dx \cong \int_a^b f_n(x)\,dx \tag{21.1}$$

where $f_n(x)$ = a polynomial of the form

$$f_n(x) = a_0 + a_1 x + \cdots + a_{n-1}x^{n-1} + a_n x^n$$

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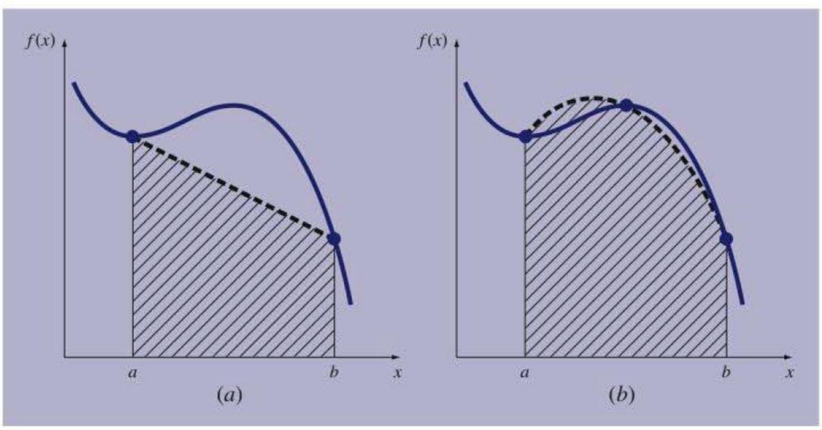

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THE TRAPEZOIDAL RULE

The *trapezoidal rule* is the first of the Newton-Cotes closed integration formulas. It corresponds to the case where the polynomial in Eq. (21.1) is first-order:

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

Recall from Chap. 18 that a straight line can be represented as [Eq. (18.2)]

$$f_1(x) = f(a) + \frac{f(b) - f(a)}{b - a}(x - a) \qquad (21.2)$$

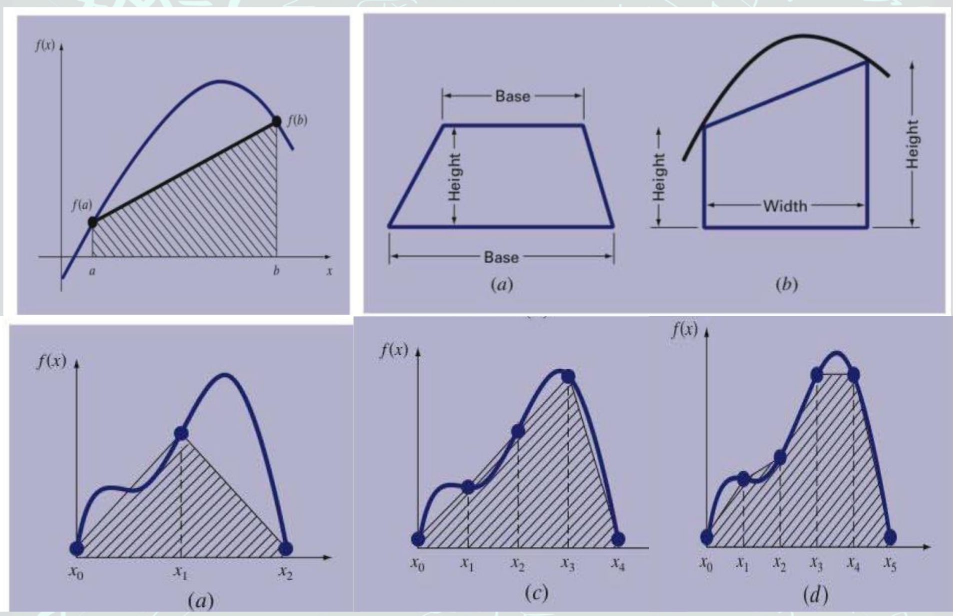
The area under this straight line is an estimate of the integral of $f(x)$ between the limits a and b:

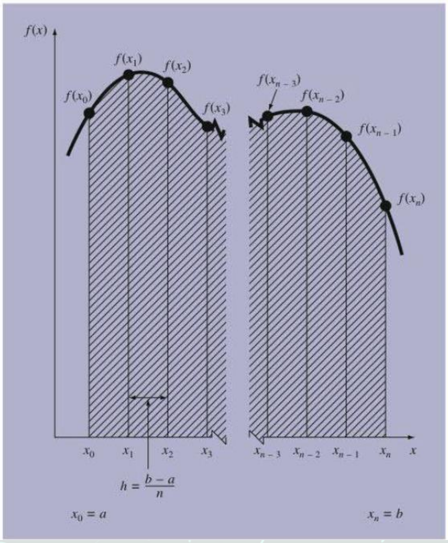
$$I = \int_a^b \left[f(a) + \frac{f(b) - f(a)}{b - a}(x - a) \right] dx$$

The result of the integration (see Box 21.1 for details) is

$$I = (b - a)\frac{f(a) + f(b)}{2} \qquad (21.3)$$

which is called the *trapezoidal rule.*





$$I = \underbrace{(b-a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)}{2n}}_{\text{Average height}}$$

(a) Single-segment

```
FUNCTION Trap (h, f0, f1)
  Trap = h * (f0 + f1)/2
END Trap
```

(b) Multiple-segment

```
FUNCTION Trapm (h, n, f)
  sum = f0
  DOFOR i = 1, n - 1
    sum = sum + 2 * fi
  END DO
  sum = sum + fn
  Trapm = h * sum / 2
END Trapm
```

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SIMPSON'S RULES

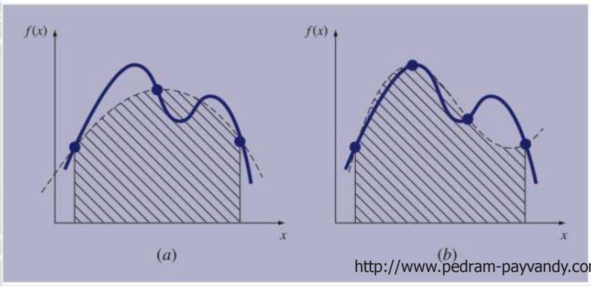
Simpson's 1/3 Rule

Simpson's 1/3 rule results when a second-order interpolating polynomial is substituted into Eq. (21.1):

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

If a and b are designated as x_0 and x_2 and $f_2(x)$ is represented by a second-order Lagrange polynomial [Eq. (18.23)], the integral becomes

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



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

$$I \cong \underbrace{(b-a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}}_{\text{Average height}}$$

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The Multiple-Application Simpson's 1/3 Rule

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

The total integral can be represented as

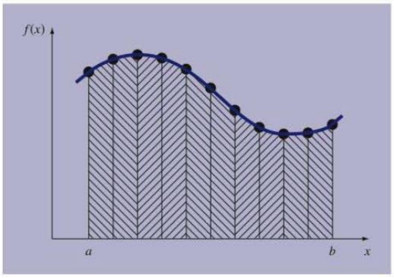
$$I = \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)\,dx$$

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

$$I \cong 2h\frac{f(x_0)+4f(x_1)+f(x_2)}{6} + 2h\frac{f(x_2)+4f(x_3)+f(x_4)}{6} + \cdots + 2h\frac{f(x_{n-2})+4f(x_{n-1})+f(x_n)}{6}$$

or, combining terms and using Eq. (21.17),

$$I \cong \underbrace{(b-a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n)}{3n}}_{\text{Average height}}$$



21.2.3 Simpson's 3/8 Rule

In a similar manner to the derivation of the trapezoidal and Simpson's 1/3 rule, a third-order Lagrange polynomial can be fit to four points and integrated:

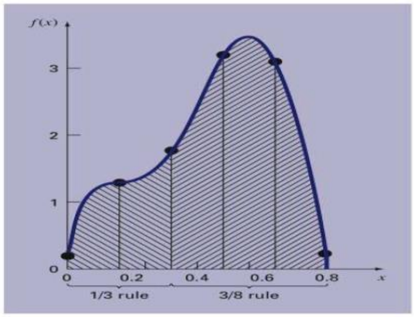
$$I = \int_a^b f(x)\,dx \cong \int_a^b f_3(x)\,dx$$

to yield

$$I \cong \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]$$

where $h = (b-a)/3$. This equation is called *Simpson's* 3/8 *rule* because h is multiplied by 3/8. It is the third Newton-Cotes closed integration formula. The 3/8 rule can also be expressed in the form of Eq. (21.5):

$$I \cong \underbrace{(b-a)}_{\text{Width}} \underbrace{\frac{f(x_0)+3f(x_1)+3f(x_2)+f(x_3)}{8}}_{\text{Average height}} \tag{21.20}$$



(a)
```
FUNCTION Simp13 (h, f0, f1, f2)
  Simp13 = 2*h* (f0+4*f1+f2) / 6
END Simp13
```

(b)
```
FUNCTION Simp38 (h, f0, f1, f2, f3)
  Simp38 = 3*h* (f0+3*(f1+f2)+f3) / 8
END Simp38
```

(c)
```
FUNCTION Simp13m (h, n, f)
  sum = f(0)
  DOFOR i = 1, n − 2, 2
    sum = sum + 4 * f_i + 2 * f_i+1
  END DO
  sum = sum + 4 * f_n-1 + f_n
  Simp13m = h * sum / 3
END Simp13m
```

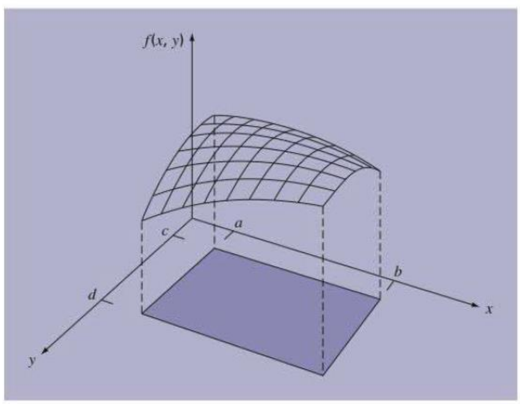
(d)
```
FUNCTION SimpInt(a,b,n,f)
  h = (b − a) / n
  IF n = 1 THEN
    sum = Trap(h, f_n−1, f_n)
  ELSE
    m = n
    odd = n / 2 − INT(n / 2)
    IF odd > 0 AND n > 1 THEN
      sum = sum+Simp38(h, f_n−3, f_n−2, f_n−1, f_n)
      m = n − 3
    END IF
    IF m > 1 THEN
      sum = sum + Simp13m(h,m,f)
    END IF
  END IF
  SimpInt = sum
END SimpInt
```

MULTIPLE INTEGRALS

Multiple integrals are widely used in engineering. For example, a general equation to compute the average of a two-dimensional function can be written as (recall Eq. PT6.4)

$$\bar{f} = \frac{\int_c^d \left(\int_a^b f(x, y)\, dx \right) dy}{(d - c)(b - a)}$$

The numerator is called a double integral.



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The techniques discussed in this chapter (and the following chapter) can be readily employed to evaluate multiple integrals. A simple example would be to take the double integral of a function over a rectangular area (Fig. 21.16).

Recall from calculus that such integrals can be computed as iterated integrals

$$\int_c^d \left(\int_a^b f(x, y)\, dx \right) dy = \int_a^b \left(\int_c^d f(x, y)\, dy \right) dx \qquad (21.24)$$

Thus, the integral in one of the dimensions is evaluated first. The result of this first integration is integrated in the second dimension. Equation (21.24) states that the order of integration is not important.

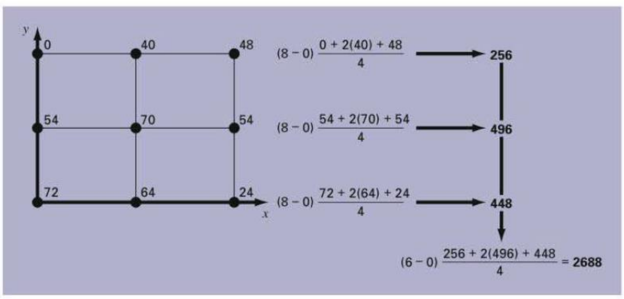
A numerical double integral would be based on the same idea. First, methods like the multiple-segment trapezoidal or Simpson's rule would be applied in the first dimension with each value of the second dimension held constant. Then the method would be applied to integrate the second dimension. The approach is illustrated in the following example.

Using Double Integral to Determine Average Temperature

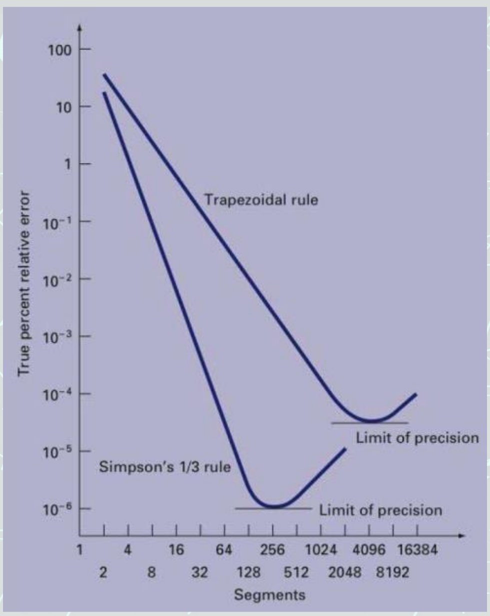
Problem Statement. Suppose that the temperature of a rectangular heated plate is described by the following function:

$$T(x, y) = 2xy + 2x - x^2 - 2y^2 + 72$$

If the plate is 8-m long (x dimension) and 6-m wide (y dimension), compute the average temperature.



Integration of Equations



$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

ROMBERG INTEGRATION

The estimate and error associated with a multiple-application trapezoidal rule can be represented generally as

$$I = I(h) + E(h)$$

where I = the exact value of the integral, $I(h)$ = the approximation from an n-segment application of the trapezoidal rule with step size $h = (b - a)/n$, and $E(h)$ = the truncation error. If we make two separate estimates using step sizes of h_1 and h_2 and have exact values for the error,

$$I(h_1) + E(h_1) = I(h_2) + E(h_2) \tag{22.1}$$

Now recall that the error of the multiple-application trapezoidal rule can be represented approximately by Eq. (21.13) [with $n = (b - a)/h$]:

$$E \cong -\frac{b-a}{12} h^2 \bar{f}'' \tag{22.2}$$

If it is assumed that $\bar{f}''$ is constant regardless of step size, Eq. (22.2) can be used to determine that the ratio of the two errors will be

$$\frac{E(h_1)}{E(h_2)} \cong \frac{h_1^2}{h_2^2} \tag{22.3}$$

This calculation has the important effect of removing the term $\bar{f}''$ from the computation. In so doing, we have made it possible to utilize the information embodied by Eq. (22.2) without prior knowledge of the function's second derivative. To do this, we rearrange Eq. (22.3) to give

$$E(h_1) \cong E(h_2)\left(\frac{h_1}{h_2}\right)^2$$

which can be substituted into Eq. (22.1):

$$I(h_1) + E(h_2)\left(\frac{h_1}{h_2}\right)^2 \cong I(h_2) + E(h_2)$$

which can be solved for

$$E(h_2) \cong \frac{I(h_1) - I(h_2)}{1 - (h_1/h_2)^2}$$

Thus, we have developed an estimate of the truncation error in terms of the integral estimates and their step sizes. This estimate can then be substituted into

$$I = I(h_2) + E(h_2)$$

to yield an improved estimate of the integral:

$$I \cong I(h_2) + \frac{1}{(h_1/h_2)^2 - 1}[I(h_2) - I(h_1)] \tag{22.4}$$

It can be shown (Ralston and Rabinowitz, 1978) that the error of this estimate is $O(h^4)$. Thus, we have combined two trapezoidal rule estimates of $O(h^2)$ to yield a new estimate of $O(h^4)$. For the special case where the interval is halved ($h_2 = h_1/2$), this equation becomes

$$I \cong I(h_2) + \frac{1}{2^2 - 1}[I(h_2) - I(h_1)]$$

or, collecting terms,

$$I \cong \frac{4}{3}I(h_2) - \frac{1}{3}I(h_1) \tag{22.5}$$

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Error Corrections of the Trapezoidal Rule

Problem Statement. In the previous chapter (Example 21.1 and Table 21.1), we used a variety of numerical integration methods to evaluate the integral of $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ from $a = 0$ to $b = 0.8$. For example, single and multiple applications of the trapezoidal rule yielded the following results:

Segments	h	Integral	ε_t, %
1	0.8	0.1728	89.5
2	0.4	1.0688	34.9
4	0.2	1.4848	9.5

Use this information along with Eq. (22.5) to compute improved estimates of the integral.

Solution. The estimates for one and two segments can be combined to yield

$$I \cong \frac{4}{3}(1.0688) - \frac{1}{3}(0.1728) = 1.367467$$

The error of the improved integral is $E_t = 1.640533 - 1.367467 = 0.273067$ ($\varepsilon_t = 16.6\%$), which is superior to the estimates upon which it was based.

In the same manner, the estimates for two and four segments can be combined to give

$$I \cong \frac{4}{3}(1.4848) - \frac{1}{3}(1.0688) = 1.623467$$

which represents an error of $E_t = 1.640533 - 1.623467 = 0.017067$ ($\varepsilon_t = 1.0\%$).

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Higher-Order Error Correction of Integral Estimates

$$I_{j,k} \cong \frac{4^{k-1} I_{j+1,k-1} - I_{j,k-1}}{4^{k-1} - 1}$$

where $I_{j+1,k-1}$ and $I_{j,k-1}$ = the more and less accurate integrals, respectively, and $I_{j,k}$ = the improved integral. The index k signifies the level of the integration, where $k = 1$ corresponds to the original trapezoidal rule estimates, $k = 2$ corresponds to $O(h^4)$, $k = 3$ to $O(h^6)$, and so forth. The index j is used to distinguish between the more $(j + 1)$ and the less (j) accurate estimates. For example, for $k = 2$ and $j = 1$, Eq. (22.8) becomes

$$I_{1,2} \cong \frac{4I_{2,1} - I_1}{3} \qquad |\varepsilon_a| = \left|\frac{I_{1,k} - I_{2,k-1}}{I_{1,k}}\right| 100\%$$

	$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$
(a)	0.172800	1.367467		
	1.068800			
(b)	0.172800	1.367467	1.640533	
	1.068800	1.623467		
	1.484800			
(c)	0.172800	1.367467	1.640533	1.640533
	1.068800	1.623467	1.640533	
	1.484800	1.639467		
	1.600800			


```
FUNCTION Romberg (a, b, maxit, es)
  LOCAL I(10, 10)
  n = 1
  I_1,1 = TrapEq(n, a, b)
  iter = 0
  DO
    iter = iter + 1
    n = 2^iter
    I_iter+1,1 = TrapEq(n, a, b)
    DOFOR k = 2, iter + 1
      j = 2 + iter - k
      I_j,k = (4^(k-1) * I_j+1,k-1 - I_j,k-1) / (4^(k-1) - 1)
    END DO
    ea = ABS((I_1,iter+1 - I_2,iter) / I_1,iter+1) * 100
    IF (iter ≥ maxit OR ea ≤ es) EXIT
  END DO
  Romberg = I_1,iter+1
END Romberg
```

FIGURE 22.4
Pseudocode for Romberg integration that uses the equal-size-segment version of the trapezoidal rule from Fig. 22.1.

ADAPTIVE QUADRATURE

The theoretical basis of the approach can be illustrated for an interval $x = a$ to $x = b$ with a width of $h_1 = b - a$. A first estimate of the integral can be estimated with Simpson's 1/3 rule,

$$I(h_1) = \frac{h_1}{6}(f(a) + 4f(c) + f(b)) \quad (22.10)$$

where $c = (a + b)/2$.

As in Richardson extrapolation, a more refined estimate can be obtained by halving the step size. That is, by applying the multiple-application Simpson's 1/3 rule with $n = 4$,

$$I(h_2) = \frac{h_2}{6}(f(a) + 4f(d) + 2f(c) + 4f(e) + f(b)) \quad (22.11)$$

where $d = (a + c)/2$, $e = (c + b)/2$, and $h_2 = h_1/2$.

Because both $I(h_1)$ and $I(h_2)$ are estimates of the same integral, their difference provides a measure of the error. That is,

$$E \cong I(h_2) - I(h_1) \quad (22.12)$$

In addition, the estimate and error associated with either application can be represented generally as

$$I = I(h) + E(h) \quad (22.13)$$

where I = the exact value of the integral, $I(h)$ = the approximation from an n-segment application of the Simpson's 1/3 rule with step size $h = (b - a)/n$, and $E(h)$ = the corresponding truncation error.

the error of the more refined estimate, $I(h_2)$, as a function of the difference between the two integral estimates,

$$E(h_2) = \frac{1}{15}[I(h_2) - I(h_1)] \quad (22.14)$$

The error can then be added to $I(h_2)$ to generate an even better estimate

$$I = I(h_2) + \frac{1}{15}[I(h_2) - I(h_1)] \quad (22.15)$$

```
FUNCTION quadapt(a, b)              (main calling function)
tol = 0.000001
c = (a + b)/2                            (initialization)
fa = f(a)
fc = f(c)
fb = f(b)
quadapt = qstep(a, b, tol, fa, fc, fb)
END quadapt

FUNCTION qstep(a, b, tol, fa, fc, fb) (recursive function)
h1 = b − a
h2 = h1/2
c = (a + b)/2
fd = f((a + c)/2)
fe = f((c + b)/2)
I1 = h1/6 * (fa + 4 * fc + fb)        (Simpson's 1/3 rule)
I2 = h2/6 * (fa + 4 * fd + 2 * fc + 4 * fe + fb)
IF |I2 − I1| ≤ tol THEN      (terminate after Boole's rule)
  I = I2 + (I2 − I1)/15
ELSE                           (recursive calls if needed)
  Ia = qstep(a, c, tol, fa, fd, fc)
  Ib = qstep(c, b, tol, fc, fe, fb)
  I = Ia + Ib
END IF
qstep = I
END qstep
```

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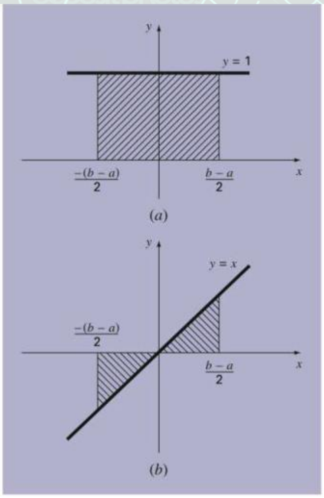
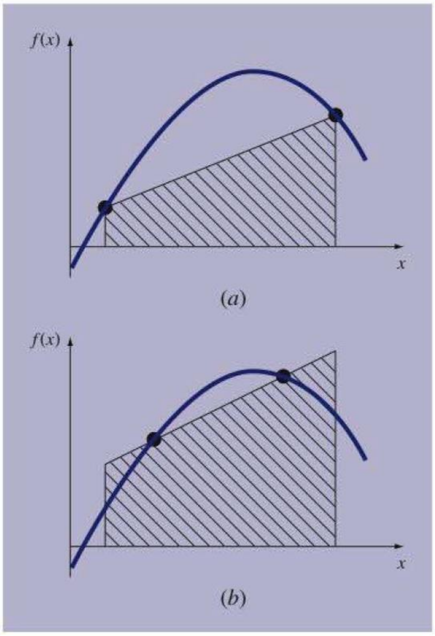
GAUSS QUADRATURE

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





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To illustrate the approach, Eq. (22.16) is expressed as

$$I \cong c_0 f(a) + c_1 f(b) \tag{22.17}$$

where the c's = constants. Now realize that the trapezoidal rule should yield exact results when the function being integrated is a constant or a straight line. Two simple equations that represent these cases are $y = 1$ and $y = x$. Both are illustrated in Fig. 22.7. Thus, the following equalities should hold:

$$c_0 + c_1 = \int_{-(b-a)/2}^{(b-a)/2} 1\, dx$$

and

$$-c_0 \frac{b-a}{2} + c_1 \frac{b-a}{2} = \int_{-(b-a)/2}^{(b-a)/2} x\, dx$$

or, evaluating the integrals,

$$c_0 + c_1 = b - a$$

and

$$-c_0 \frac{b-a}{2} + c_1 \frac{b-a}{2} = 0$$

These are two equations with two unknowns that can be solved for

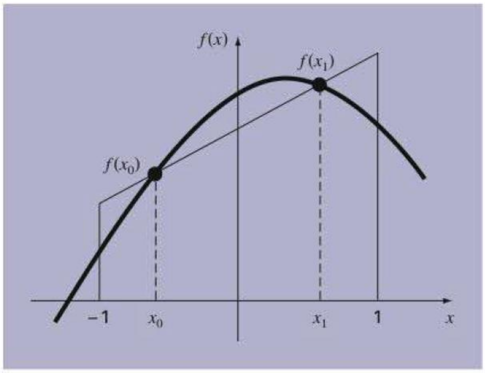
$$c_0 = c_1 = \frac{b-a}{2}$$

22.4.2 Derivation of the Two-Point Gauss-Legendre Formula

Just as was the case for the above derivation of the trapezoidal rule, the object of Gauss quadrature is to determine the coefficients of an equation of the form

$$I \cong c_0 f(x_0) + c_1 f(x_1) \tag{22.18}$$

where the c's = the unknown coefficients. However, in contrast to the trapezoidal rule that used fixed end points a and b, the function arguments x_0 and x_1 are not fixed at the end points, but are unknowns (Fig. 22.8). Thus, we now have a total of four unknowns that must be evaluated, and consequently, we require four conditions to determine them exactly.



Just as for the trapezoidal rule, we can obtain two of these conditions by assuming that Eq. (22.18) fits the integral of a constant and a linear function exactly. Then, to arrive at the other two conditions, we merely extend this reasoning by assuming that it also fits the integral of a parabolic ($y = x^2$) and a cubic ($y = x^3$) function. By doing this, we determine all four unknowns and in the bargain derive a linear two-point integration formula that is exact for cubics. The four equations to be solved are

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} 1\, dx = 2 \tag{22.19}$$

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x\, dx = 0 \tag{22.20}$$

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x^2\, dx = \frac{2}{3} \tag{22.21}$$

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x^3\, dx = 0 \tag{22.22}$$

Equations (22.19) through (22.22) can be solved simultaneously for

$$c_0 = c_1 = 1$$

$$x_0 = -\frac{1}{\sqrt{3}} = -0.5773503\ldots$$

$$x_1 = \frac{1}{\sqrt{3}} = 0.5773503\ldots$$

which can be substituted into Eq. (22.18) to yield the two-point Gauss-Legendre formula

$$I \cong f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \tag{22.23}$$

Thus, we arrive at the interesting result that the simple addition of the function values at $x = 1/\sqrt{3}$ and $-1/\sqrt{3}$ yields an integral estimate that is third-order accurate.

Notice that the integration limits in Eqs. (22.19) through (22.22) are from -1 to 1. This was done to simplify the mathematics and to make the formulation as general as possible. A simple change of variable can be used to translate other limits of integration into this form. This is accomplished by assuming that a new variable x_d is related to the original variable x in a linear fashion, as in

$$x = a_0 + a_1 x_d \tag{22.24}$$

If the lower limit, $x = a$, corresponds to $x_d = -1$, these values can be substituted into Eq. (22.24) to yield

$$a = a_0 + a_1(-1) \tag{22.25}$$

Similarly, the upper limit, $x = b$, corresponds to $x_d = 1$, to give

$$b = a_0 + a_1(1) \tag{22.26}$$

Equations (22.25) and (22.26) can be solved simultaneously for

$$a_0 = \frac{b+a}{2} \tag{22.27}$$

and

$$a_1 = \frac{b-a}{2} \tag{22.28}$$

which can be substituted into Eq. (22.24) to yield

$$x = \frac{(b+a)+(b-a)x_d}{2} \tag{22.29}$$

This equation can be differentiated to give

$$dx = \frac{b-a}{2}\,dx_d \tag{22.30}$$

Equations (22.29) and (22.30) can be substituted for x and dx, respectively, in the equation to be integrated. These substitutions effectively transform the integration interval without changing the value of the integral. The following example illustrates how this is done in practice.

Two-Point Gauss-Legendre Formula

Problem Statement. Use Eq. (22.23) to evaluate the integral of

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

between the limits $x = 0$ to 0.8. Recall that this was the same problem that we solved in Chap. 21 using a variety of Newton-Cotes formulations. The exact value of the integral is 1.640533.

Solution. Before integrating the function, we must perform a change of variable so that the limits are from −1 to +1. To do this, we substitute $a = 0$ and $b = 0.8$ into Eq. (22.29) to yield

$$x = 0.4 + 0.4x_d$$

The derivative of this relationship is [Eq. (22.30)]

$$dx = 0.4\,dx_d$$

Both of these can be substituted into the original equation to yield

$$\int_0^{0.8} (0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5)\,dx$$
$$= \int_{-1}^{1} \big[0.2 + 25(0.4+0.4x_d) - 200(0.4+0.4x_d)^2 + 675(0.4+0.4x_d)^3 - 900(0.4+0.4x_d)^4 + 400(0.4+0.4x_d)^5\big]0.4\,dx_d$$

Therefore, the right-hand side is in the form that is suitable for evaluation using Gauss quadrature. The transformed function can be evaluated at $-1/\sqrt{3}$ to be equal to

0.516741 and at $1/\sqrt{3}$ to be equal to 1.305837. Therefore, the integral according to Eq. (22.23) is

$$I \cong 0.516741 + 1.305837 = 1.822578$$

which represents a percent relative error of −11.1 percent. This result is comparable in magnitude to a four-segment application of the trapezoidal rule (Table 21.1) or a single application of Simpson's 1/3 and 3/8 rules (Examples 21.4 and 21.6). This latter result is to be expected because Simpson's rules are also third-order accurate. However, because of the clever choice of base points, Gauss quadrature attains this accuracy on the basis of only two function evaluations.