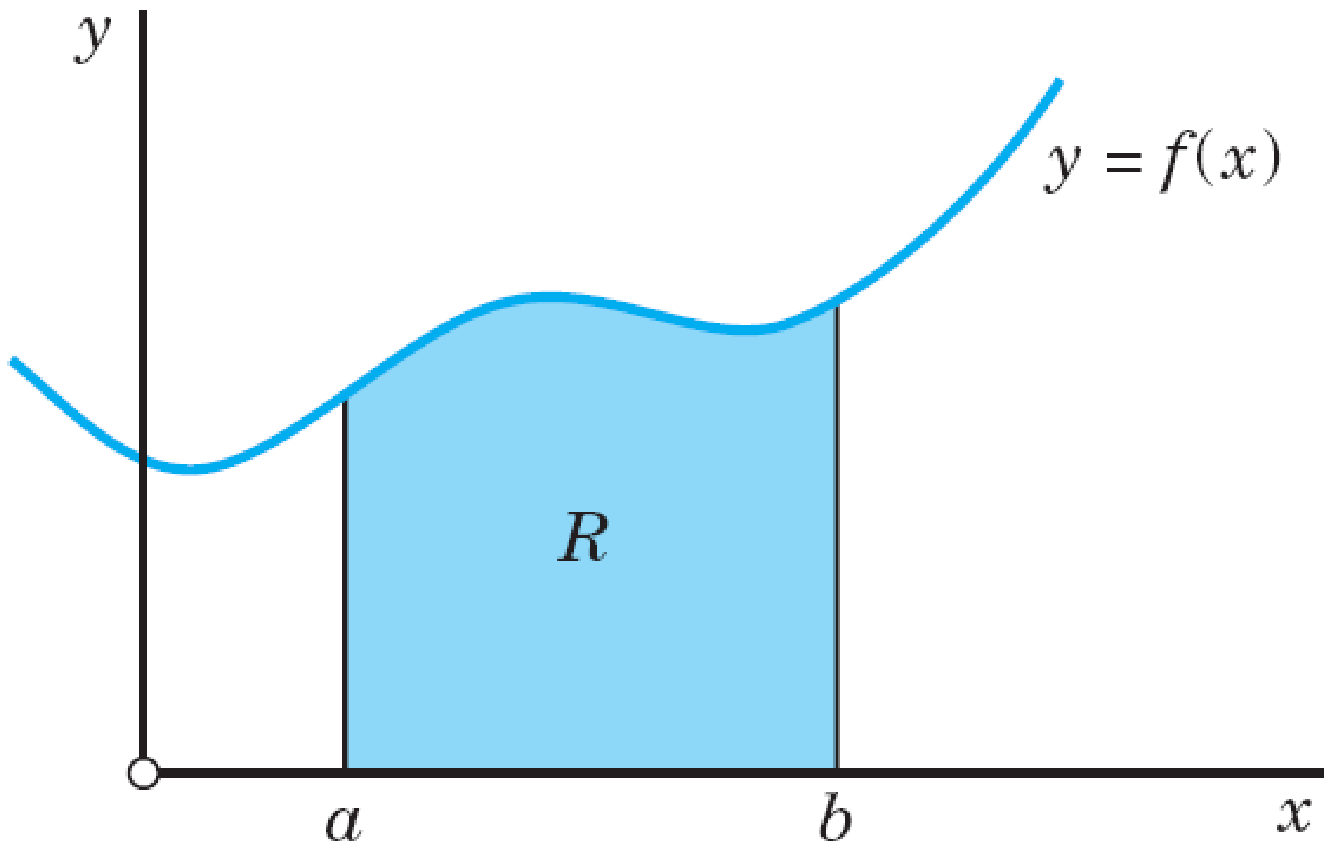
19.5 Numeric Integration and Differentiation

- Applications often lead to integrals whose analytic evaluation would be very difficult or even impossible, or whose integrand is an empirical function given by recorded numeric values. Then we may obtain approximate numeric values of the integral by a numeric integration method.

continued

Fig. 437. Geometric interpretation of a definite integral



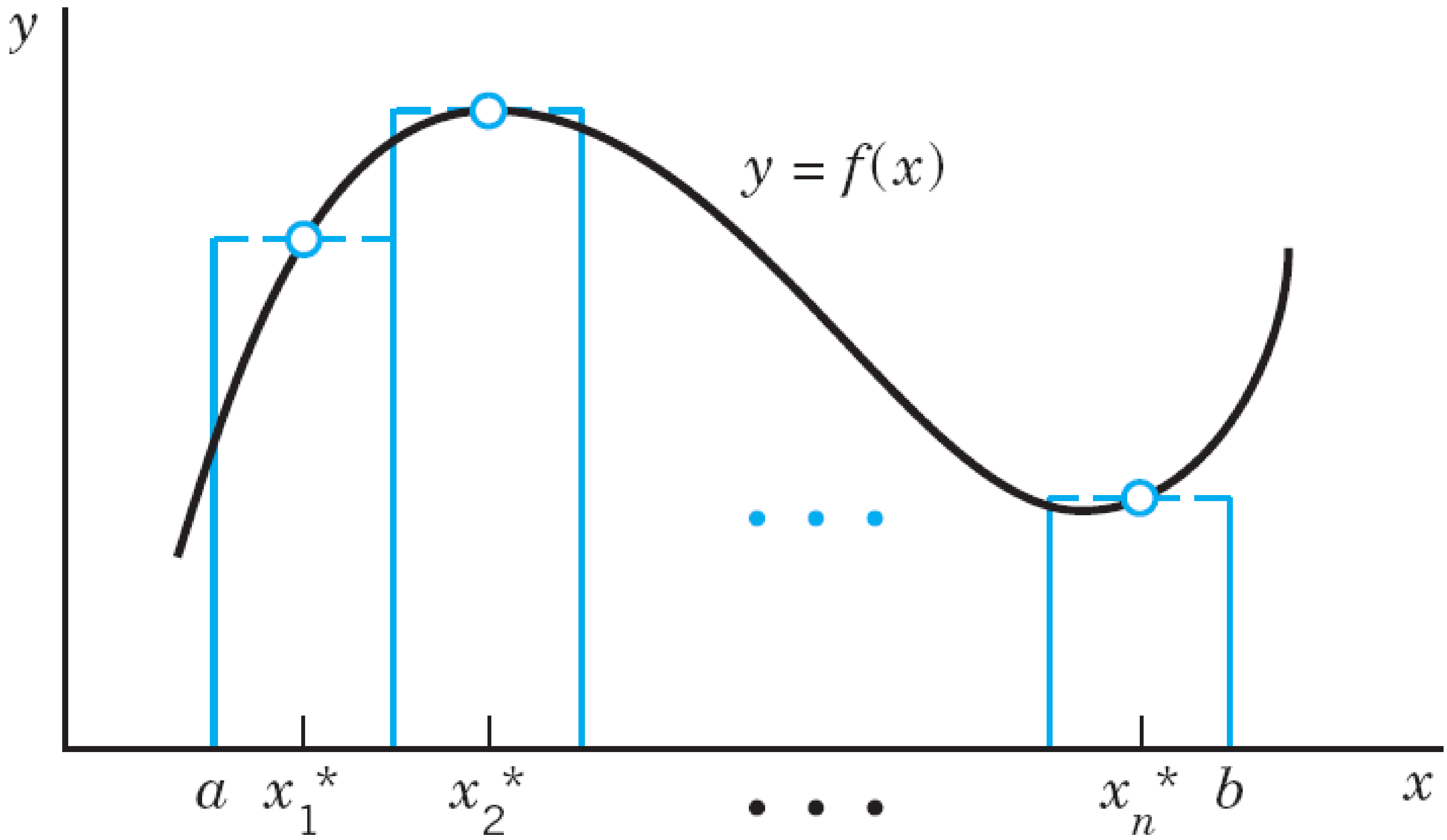
Rectangular Rule. Trapezoidal Rule

- The simplest formula, the **rectangular rule,** is obtained if we subdivide the interval of integration $a \le x \le b$ into n subintervals of equal length $h = (b - a)/n$ and in each subinterval approximate f by the constant $f(x_j^*)$, the value of f at the midpoint x_j^* of the jth subinterval (Fig. 438). Then f is approximated by a **step function** (piecewise constant function), the n rectangles in Fig. 438 have the areas $f(x_1^*)h$, ..., $f(x_n^*)h$, and the **rectangular rule** is

(1) $$J = \int_a^b f(x)\,dx \approx h[f(x_1^*) + f(x_2^*) + \cdots + f(x_n^*)] \qquad \left(h = \frac{b-a}{n}\right).$$

continued

Fig. 438. Rectangular rule

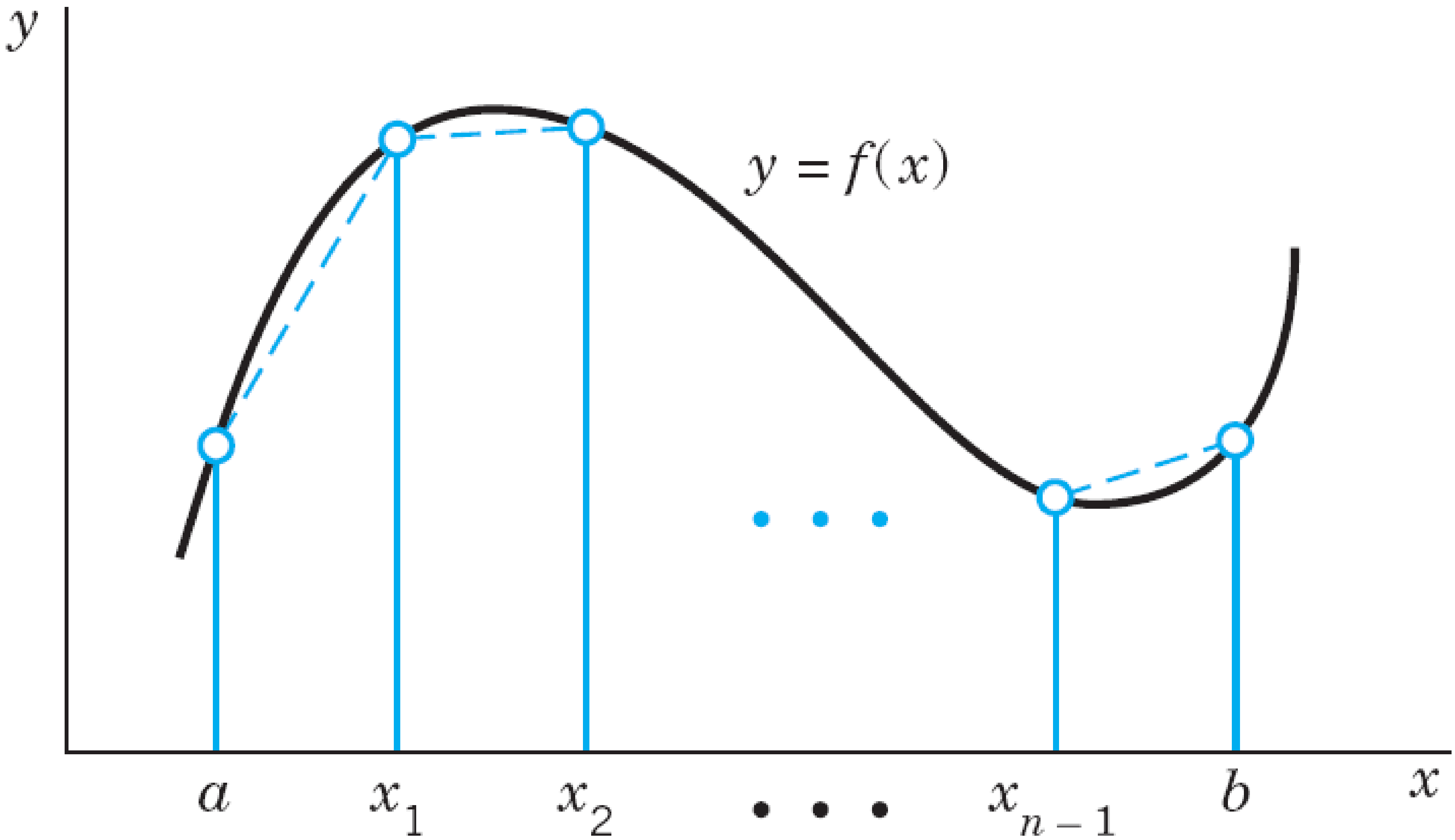


- The **trapezoidal rule** is generally more accurate. We obtain it if we take the same subdivision as before and approximate f by a broken line of segments (chords) with endpoints $[a, f(a)]$, $[x_1, f(x_1)]$, ..., $[b, f(b)]$ on the curve of f (Fig. 439). Then the area under the curve of f between a and b is approximated by n trapezoids of areas

$$\tfrac{1}{2}[f(a) + f(x_1)]h, \qquad \tfrac{1}{2}[f(x_1) + f(x_2)]h, \qquad \cdots, \qquad \tfrac{1}{2}[f(x_{n-1}) + f(b)]h.$$

continued

Fig. 439. Trapezoidal rule



EXAMPLE 1 Trapezoidal Rule

- Evaluate $J = \int_0^1 e^{-x^2}\,dx$ by means of (2) with $n = 10$.
- ***Solution.*** $J \approx 0.1(0.5 \cdot 1.367\,879 + 6.778\,167) = 0.746\,211$ from Table 19.3.

continued

Table 19.3 Computations in Example 1

j	x_j	$x_j^{\,2}$	$e^{-x_j^{\,2}}$	
0	0	0	1.000 000	
1	0.1	0.01		0.990 050
2	0.2	0.04		0.960 789
3	0.3	0.09		0.913 931
4	0.4	0.16		0.852 144
5	0.5	0.25		0.778 801
6	0.6	0.36		0.697 676
7	0.7	0.49		0.612 626
8	0.8	0.64		0.527 292
9	0.9	0.81		0.444 858
10	1.0	1.00	0.367 879	
Sums			1.367 879	6.778 167

Error Bounds and Estimate for the Trapezoidal Rule

- The **error** ε of (2) with any n is the sum of such contributions from the n subintervals; since $h = (b - a)/n$, $nh^3 = n(b - a)^3/n^3$, and $(b - a)^2 = n^2h^2$, we obtain

(3) $$\epsilon = -\frac{(b-a)^3}{12n^2} f''(\hat{t}) = -\frac{(b-a)}{12} h^2 f''(\hat{t})$$

with (suitable, unknown) $\hat{t}$ between a and b.

continued

- Because of (3) the trapezoidal rule (2) is also written

(2*) $$J = \int_a^b f(x)\,dx = h\left[\tfrac{1}{2}f(a) + f(x_1) + \cdots + f(x_{n-1}) + \tfrac{1}{2}f(b)\right] - \frac{b-a}{12}\,h^2 f''(\hat{t}).$$

- **Error Bounds** are now obtained by taking the largest value for *f*'', say, M_2, and the smallest value, M_2^*, in the interval of integration. Then (3) gives (note that *K* is negative)

(4) $$KM_2 \leqq \epsilon \leqq KM_2^* \qquad \text{where} \qquad K = -\frac{(b-a)^3}{12n^2} = -\frac{b-a}{12}\,h^2.$$

continued

- **Error Estimation by Halving *h*** is advisable if h'' is very complicated or unknown, for instance, in the case of experimental data. Then we may apply the Error Principle of Sec. 19.1. That is, we calculate by (2), first with h, obtaining, say, $J = J_h + \varepsilon_h$, and then with $1/2h$, obtaining $J = J_{h/2} + \varepsilon_{h/2}$. Now if we replace h^2 in (3) with $(1/2h)^2$, the error is multiplied by 1/4. Hence $\varepsilon_{h/2} \approx 1/4\varepsilon_h$ (not exactly because $\hat{t}$ may differ). Together, $J_{h/2} + \varepsilon_{h/2} = J_h + \varepsilon_h \approx J_h + 4\varepsilon_{h/2}$. Thus $J_{h/2} - J_h = (4 - 1)\varepsilon_{h/2}$. Division by 3 gives the error formula for $J_{h/2}$

(5)
$$\epsilon_{h/2} \approx \frac{1}{3}\,(J_{h/2} - J_h).$$

EXAMPLE 2 Error Estimation for the Trapezoidal Rule by (4) and (5)

- Estimate the error of the approximate value in Example 1 by (4) and (5).

- ***Solution.*** **(A)** ***Error bounds by*** **(4).** By differentiation, $f''(x) = 2(2x^2 - 1)e^{-x^2}$. Also, $f'''(x) > 0$ if $0 < x < 1$, so that the minimum and maximum occur at the ends of the interval. We compute $M_2 = f''(1) = 0.735\ 759$ and $M_2^* = f''(0) = -2$. Furthermore, $K = -1/1200$, and (4) gives

$$-0.000\ 614 \leqq \epsilon \leqq 0.001\ 667.$$

continued

Hence the exact value of J must lie between

$$0.746\,211 - 0.000\,614 = 0.745\,597 \qquad \text{and} \qquad 0.746\,211 + 0.001\,667 = 0.747\,878.$$

- Actually, $J = 0.746\ 824$, exact to 6D.
- **(B)** ***Error estimate by*** **(5).** $J_h = 0.746211$ in Example 1. Also,

$$J_{h/2} = 0.05\left[\sum_{j=1}^{19} e^{-(j/20)^2} + \frac{1}{2}(1 + 0.367879)\right] = 0.746671.$$

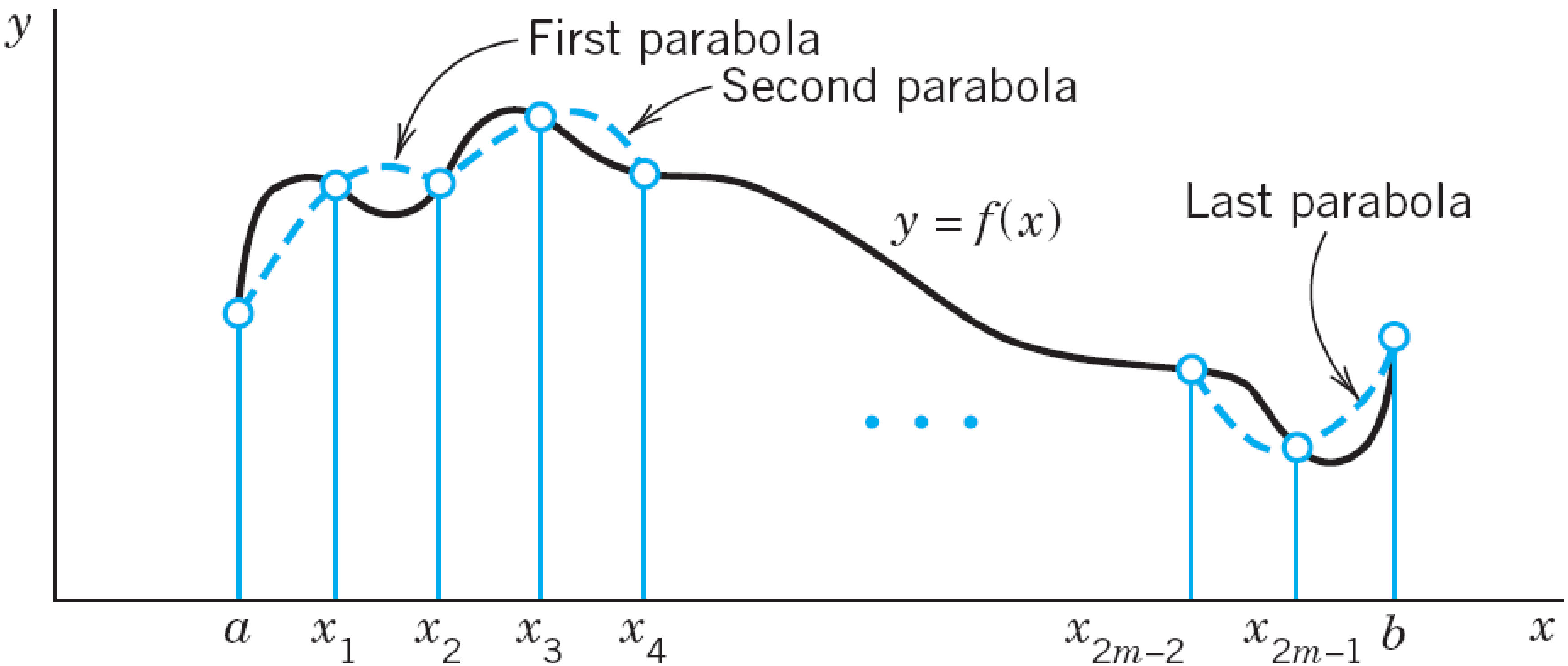
Hence $\varepsilon_{h/2} = 1/3\ (J_{h/2} - J_h) = 0.000153$ and $J_{h/2} + \varepsilon_{h/2} = 0.746824$, exact to 6D.

Simpson's Rule of Integration

- To derive Simpson's rule, we divide the interval of integration $a \le x \le b$ into an ***even number*** of equal subintervals, say, into $n = 2m$ subintervals of length $h = (b - a)/(2m)$, with endpoints x_0 $(= a)$, x_1, ..., x_{2m-1}, x_{2m} $(= b)$; see Fig. 440. We now take the first two subintervals and approximate $f(x)$ in the interval $x_0 \le x \le x_2 = x_0 + 2h$ by the Lagrange polynomial $p_2(x)$ through (x_0, f_0), (x_1, f_1), (x_2, f_2), where $f_j = f(x_j)$.

continued

Fig. 440. Simpson's rule



- We obtain **Simpson's rule**

(7) $$\int_a^b f(x)\,dx \approx \frac{h}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + \cdots + 2f_{2m-2} + 4f_{2m-1} + f_{2m}\right),$$

where $h = (b - a)/(2m)$ and $f_j = f(x_j)$. Table 19.4 shows an algorithm for Simpson's rule.

Table 19.4 Simpson's Rule of Integration

ALGORITHM SIMPSON $(a, b, m, f_0, f_1, \cdots, f_{2m})$

This algorithm computes the integral $J = \int_a^b f(x)\,dx$ from given values $f_j = f(x_j)$ at equidistant $x_0 = a$, $x_1 = x_0 + h, \cdots, x_{2m} = x_0 + 2mh = b$ by Simpson's rule (7), where $h = (b - a)/(2m)$.

INPUT: $a, b, m, f_0, \cdots, f_{2m}$

OUTPUT: Approximate value $\tilde{J}$ of J

Compute $s_0 = f_0 + f_{2m}$

$$s_1 = f_1 + f_3 + \cdots + f_{2m-1}$$

$$s_2 = f_2 + f_4 + \cdots + f_{2m-2}$$

$$h = (b - a)/2m$$

$$\tilde{J} = \frac{h}{3}(s_0 + 4s_1 + 2s_2)$$

OUTPUT $\tilde{J}$. Stop.

End SIMPSON

★ **Error of Simpson's Rule (7).** If the fourth derivative $f^{(4)}$ exists and is continuous on $a \leq x \leq b$, the **error** of (7), call it ε_S, is

(8) $$\epsilon_S = -\frac{(b-a)^5}{180(2m)^4} f^{(4)}(\hat{t}) = -\frac{(b-a)}{180} h^4 f^{(4)}(\hat{t});$$

here $\hat{t}$ is a suitable unknown value between a and b. This is obtained similarly to (3). With this we may also write Simpson's rule (7) as

continued

(7)** $$\int_a^b f(x)\,dx = \frac{h}{3}(f_0 + 4f_1 + \cdots + f_{2m}) - \frac{(b-a)}{180} h^4 f^{(4)}(\hat{t}).$$

★ **Error Bounds.** By taking for $f^{(4)}$ in (8) the maximum M_4 and minimum $M_4{}^*$ on the interval of integration we obtain from (8) the error bounds (note that C is negative)

(9) $$CM_4 \leqq \epsilon_S \leqq CM_4{}^* \qquad \text{where} \qquad C = -\frac{(b-a)^5}{180(2m)^4} = -\frac{(b-a)}{180} h^4.$$

- **Numeric Stability** *with respect to rounding* is another important property of Simpson's rule. Indeed, for the sum of the roundoff errors *j* of the 2*m* + 1 values *f j* in (7) we obtain, since *h* = (*b* – *a*)/2*m*,

$$\frac{h}{3}\left|\epsilon_0 + 4\epsilon_1 + \cdots + \epsilon_{2m}\right| \leqq \frac{(b-a)}{3 \cdot 2m} 6mu = (b-a)u$$

continued

where u is the rounding unit ($u = 1/2 \cdot 10^{-6}$ if we round off to 6D; see Sec. 19.1). Also $6 = 1 + 4 + 1$ is the sum of the coefficients for a pair of intervals in (7); take $m = 1$ in (7) to see this. The bound $(b - a)u$ is independent of m, so that it cannot increase with increasing m, that is, with decreasing h. This proves stability.

EXAMPLE3 Simpson's Rule. Error Estimate

- Evaluate $J = \int_0^1 e^{-x^2}\,dx$ by Simpson's rule with 2*m* = 10 and estimate the error.
- ***Solution.*** Since *h* = 0.1, Table 19.5 gives

$$J \approx \frac{0.1}{3}\,(1.367\,879 + 4 \cdot 3.740\,266 + 2 \cdot 3.037\,901) = 0.746\,825.$$

continued

- *Estimate of error.* Differentiation gives $f^{(4)}(x) = 4(4x^4 - 12x^2 + 3)e^{-x^2}$. By considering the derivative $f^{(5)}$ of $f^{(4)}$ we find that the largest value of $f^{(4)}$ in the interval of integration occurs at 0 and the smallest value at $x^* = (2.5 - 0.5\sqrt{10})^{1/2}$. Computation gives the values $M_4 = f^{(4)}(0) = 12$ and $M_4^* = f^{(4)}(x^*) = -7.419$. Since $2m = 10$ and $b - a = 1$, we obtain $C = -1/1\,800\,000 = -0.000\,000\,56$. Therefore, from (9),

$$-0.000\,007 \leqq \epsilon_S \leqq 0.000\,005.$$

continued

- Hence J must lie between 0.746 825 – 0.000 007 = 0.746 818 and 0.746 825 + 0.000 005 = 0.746 830, so that at least four digits of our approximate value are exact. Actually, the value 0.746 825 is exact to 5D because J = 0.746 824 (exact to 6D).
- Thus our result is much better than that in Example 1 obtained by the trapezoidal rule, whereas the number of operations is nearly the same in both cases.

continued

Table 19.5 Computations in Example 3

j	x_j	$x_j^{\,2}$	$e^{-x_j^{\,2}}$		
0	0	0	1.000 000		
1	0.1	0.01		0.990 050	
2	0.2	0.04			0.960 789
3	0.3	0.09		0.913 931	
4	0.4	0.16			0.852 144
5	0.5	0.25		0.778 801	
6	0.6	0.36			0.697 676
7	0.7	0.49		0.612 626	
8	0.8	0.64			0.527 292
9	0.9	0.81		0.444 858	
10	1.0	1.00	0.367 879		
Sums			1.367 879	3.740 266	3.037 901

EXAMPLE4 Determination of $n = 2m$ in Simpson's Rule from the Required Accuracy

- What n should we choose in Example 3 to get 6D-accuracy?
- ***Solution.*** Using $M_4 = 12$ (which is bigger in absolute value than M_4^*), we get from (9), with $b - a = 1$ and the required accuracy,

$$|CM_4| = \frac{12}{180(2m)^4} = \frac{1}{2} \cdot 10^{-6}, \qquad \text{thus} \qquad m = \left[\frac{2 \cdot 10^6 \cdot 12}{180 \cdot 2^4}\right]^{1/4} = 9.55.$$

  Hence we should choose $n = 2m = 20$. Do the computation, which parallels that in Example 3.
- Note that the error bounds in (4) or (9) may sometimes be loose, so that in such a case a smaller $n = 2m$ may already suffice.

EXAMPLE5 Error Estimation for Simpson's Rule by Halving

- Integrate $f(x) = 1/4\pi x^4 \cos 1/4\pi x$ from 0 to 2 with $h = 1$ and apply (10).
- ***Solution.*** The exact 5D-value of the integral is $J = 1.25953$. Simpson's rule gives

$$J_h = \tfrac{1}{3}[f(0) + 4f(1) + f(2)] = \tfrac{1}{3}(0 + 4 \cdot 0.555360 + 0) = 0.740480,$$

$$J_{h/2} = \frac{1}{6}\left[f(0) + 4f\left(\frac{1}{2}\right) + 2f(1) + 4f\left(\frac{3}{2}\right) + f(2)\right]$$

$$= \frac{1}{6}[0 + 4 \cdot 0.045351 + 2 \cdot 0.555361 + 4 \cdot 1.521579 + 0] = 1.22974.$$

continued

- Hence (10) gives $\varepsilon_{h/2} = 1/15(1.22974 - 0.74048) = 0.032617$ and thus $J \approx J_{h/2} + \varepsilon_{h/2} = 1.26236$, with an error -0.00283, which is less in absolute value than 1/10 of the error 0.02979 of $J_{h/2}$. Hence the use of (10) was well worthwhile.

Adaptive Integration

- The idea is to adapt step h to the variability of $f(x)$. That is, where f varies but little, we can proceed in large steps without causing a substantial error in the integral, but where f varies rapidly, we have to take small steps in order to stay everywhere close enough to the curve of f.

EXAMPLE 6 Adaptive Integration with Simpson's Rule

- Integrate $f(x) = 1/4\pi x^4 \cos 1/4\pi x$ from $x = 0$ to 2 by adaptive integration and with Simpson's rule and TOL[0, 2] = 0.0002.

- ***Solution.*** Table 19.6 shows the calculations. Figure 441 shows the integrand $f(x)$ and the adapted intervals used. The first two intervals ([0, 0.5], [0.5, 1.0]) have length 0.5, hence $h = 0.25$ [because we use $2m = 2$ subintervals in Simpson's rule (7**)]. The next two intervals ([1.00, 1.25], [1.25, 1.50]) have length 0.25 (hence $h = 0.125$) and the last four intervals have length 0.125.

continued

- *Sample computations.* For 0.740480 see Example 5. Formula (10) gives (0.123716 – 0.122794)/15 = 0.000061. Note that 0.123716 refers to [0, 0.5] and [0.5, 1], so that we must subtract the value corresponding to [0, 1] in the line before. Etc. TOL[0, 2] = 0.0002 gives 0.0001 for subintervals of length 1, 0.00005 for length 0.5, etc. The value of the integral obtained is the sum of the values marked by an asterisk (for which the error estimate has become less than TOL). This gives

$$J \approx 0.123716 + 0.528895 + 0.388263 + 0.218483 = 1.25936.$$

continued

- The exact 5D-value is $J = 1.25953$. Hence the error is 0.00017. This is about 1/200 of the absolute value of that in Example 5. Our more extensive computation has produced a much better result.

continued

Table 19.6 Computations in Example 6

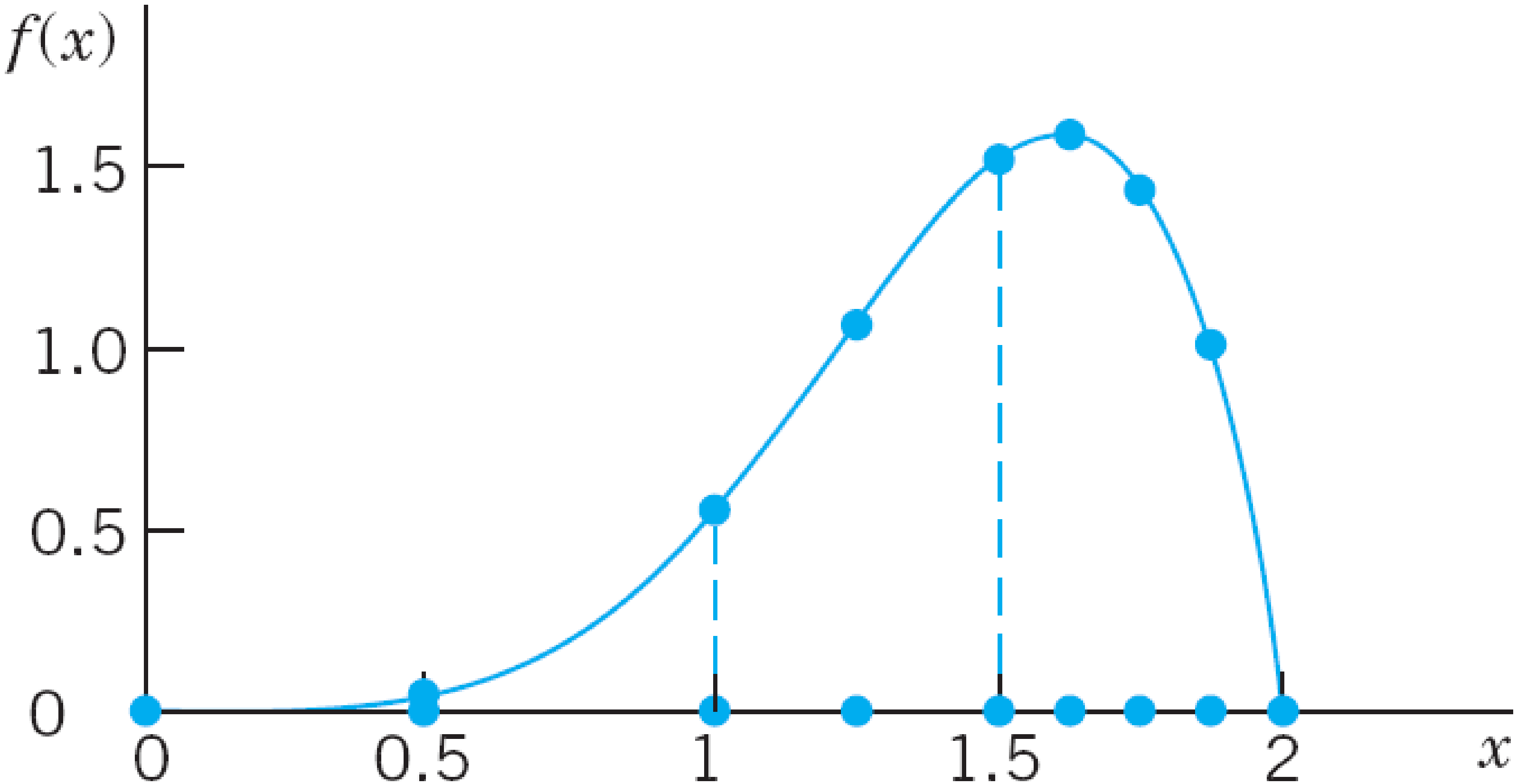
Interval	Integral	Error (10)	TOL	Comment
[0, 2]	0.740480		0.0002	
[0, 1]	0.122794			
[1, 2]	1.10695			
	Sum = 1.22974	0.032617	0.0002	Divide further
[0.0, 0.5]	0.004782			
[0.5, 1.0]	0.118934			
	Sum = 0.123716*	0.000061	0.0001	TOL reached
[1.0, 1.5]	0.528176			
[1.5, 2.0]	0.605821			
	Sum = 1.13300	0.001803	0.0001	Divide further

continued

Table 19.6 Computations in Example 6

Interval	Integral	Error (10)	TOL	Comment
[1.00, 1.25]	0.200544			
[1.25, 1.50]	0.328351			
	Sum = 0.528895*	0.000048	0.00005	TOL reached
[1.50, 1.75]	0.388235			
[1.75, 2.00]	0.218457			
	Sum = 0.606692	0.000058	0.00005	Divide further
[1.500, 1.625]	0.196244			
[1.625, 1.750]	0.192019			
	Sum = 0.388263*	0.000002	0.000025	TOL reached
[1.750, 1.875]	0.153405			
[1.875, 2.000]	0.065078			
	Sum = 0.218483*	0.000002	0.000025	TOL reached

Fig. 441. Adaptive integration in Example 6



Gauss Integration Formulas
Maximum Degree of Precision

★ (11) $$\int_{-1}^{1} f(t)\,dt \approx \sum_{j=1}^{n} A_j f_j \qquad [f_j = f(t_j)]$$

with fixed n, and $t = \pm 1$ obtained from $x = a$, b by setting $x = 1/2\,[a(t - 1) + b(t + 1)]$. Then we determine the n coefficients $A_1, \ldots., A_n$ and n nodes $t_1, \ldots., t_n$ so that (11) gives exact results for polynomials of degree k as high as possible. Since $n + n = 2n$ is the number of coefficients of a polynomial of degree $2n - 1$, it follows that $k \leq 2n - 1$.

continued

- Gauss has shown that exactness for polynomials of degree not exceeding $2n - 1$ (instead of $n - 1$ for predetermined nodes) can be attained, and he has given the location of the t_j (= the jth zero of the Legendre polynomial P_n in Sec. 5.3) and the coefficients A_j which depend on n but not on $f(t)$, and are obtained by using Lagrange's interpolation polynomial, as shown in Ref. [E5] listed in App. 1. With these t_j and A_j, formula (11) is called a **Gauss integration formula** or *Gauss quadrature formula.* Its degree of precision is $2n - 1$, as just explained. Table 19.7 gives the values needed for $n = 2, \ldots, 5$. (For larger n, see Ref. [GR1] in App. 1.)

continued

Table 19.7 Gauss Integration: Nodes t_j and Coefficients A_j

n	Nodes t_j	Coefficients A_j	Degree of Precision
2	−0.57735 02692	1	3
	0.57735 02692	1	
3	−0.77459 66692	0.55555 55556	5
	0	0.88888 88889	
	0.77459 66692	0.55555 55556	
4	−0.86113 63116	0.34785 48451	7
	−0.33998 10436	0.65214 51549	
	0.33998 10436	0.65214 51549	
	0.86113 63116	0.34785 48451	
5	−0.90617 98459	0.23692 68851	9
	−0.53846 93101	0.47862 86705	
	0	0.56888 88889	
	0.53846 93101	0.47862 86705	
	0.90617 98459	0.23692 68851	

EXAMPLE 7 Gauss Integration Formula with $n = 3$

- Evaluate the integral in Example 3 by the Gauss integration formula (11) with $n = 3$.
- ***Solution.*** We have to convert our integral from 0 to 1 into an integral from –1 to 1. We set $x = 1/2\ (t + 1)$. Then $dx = 1/2\ dt$, and (11) with $n = 3$ and the above values of the nodes and the coefficients yields

$$\int_0^1 \exp(-x^2)\, dx = \frac{1}{2}\int_{-1}^{1} \exp\left(-\frac{1}{4}(t+1)^2\right) dt$$

$$\approx \frac{1}{2}\left[\frac{5}{9}\exp\left(-\frac{1}{4}\left(1-\sqrt{\frac{3}{5}}\right)^2\right) + \frac{8}{9}\exp\left(-\frac{1}{4}\right) + \frac{5}{9}\exp\left(-\frac{1}{4}\left(1+\sqrt{\frac{3}{5}}\right)^2\right)\right] = 0.746\,815$$

continued

(exact to 6D: 0.746 825), which is almost as accurate as the Simpson result obtained in Example 3 with a much larger number of arithmetic operations. With 3 function values (as in this example) and Simpson's rule we would get 1/6 $(1 + 4e^{-0.25} + e^{-1}) = 0.747\ 180$, with an error over 30 times that of the Gauss integration.

EXAMPLE 8 Gauss Integration Formula with n = 4 and 5

- Integrate $f(x) = 1/4\pi x^4 \cos 1/4\pi x$ from $x = 0$ to 2 by Gauss. Compare with the adaptive integration in Example 6 and comment.

- ***Solution.*** $x = t + 1$ gives $f(t)\ \ 1/4\pi\,(t + 1)^4 \cos\,(1/4\pi\,(t + 1))$, as needed in (11). For $n = 4$ we calculate (6S)

$$J \approx A_1 f_1 + \cdots + A_4 f_4 = A_1(f_1 + f_4) + A_2(f_2 + f_3)$$

$$= 0.347855(0.000290309 + 1.02570) + 0.652145(0.129464 + 1.25459) = 1.25950.$$

continued

- The error is 0.00003 because J = 1.25953 (6S). Calculating with 10S and n = 4 gives the same result; so the error is due to the formula, not rounding. For n = 5 and 10S we get $J \approx 1.25952\ 6185$, too large by the amount 0.00000 0250 because J = 1.25952 5935 (10S). The accuracy is impressive, particularly if we compare the amount of work with that in Example 6.