Chapter 8

Differentiation and Integration

Given a function $f(x)$, whether known as discrete data or as continuum values, it is a classical problem to calculate the functionals $f'(x)$ or $\int_a^b f(x)$. Except for a few simple functions, it is not always possible to obtain closed form solutions. Therefore, numerical techniques for approximating these functions becomes important in practice.

8.1 Numerical Differentiation

Suppose values of $f(x)$ is known as continuum data, then the derivatives of $f(x)$ usually can be approximated by difference quotients. These formulas usually can be derived from the Taylor series representation.

Example. Suppose $f(x)$ has a Taylor's polynomial expansion near the point $x = c$. For instance, suppose $f(c+h)_= f(c) + f'(c)h + \frac{f''(c)}{2}h^2 + \frac{f'''(c)}{6}h^3 + 0(h^4)$, and $f(c-h) = f(c) - f'(c)h + \frac{f''(c)}{2}h^2 - \frac{f'''(c)}{6}h^3 + 0(h^4)$. Then

$$f'(c) = \frac{f(c+h) - f(c)}{h} + 0(h), \tag{8.1}$$

$$f'(c) = \frac{f(c+h) - f(c-h)}{2h} + 0(h^2), \tag{8.2}$$

$$f'(c) = \frac{-3f(c) + 4f(c+h) - f(c+2h)}{2h} + 0(h^2), \tag{8.3}$$

$$f''(c) = \frac{f(c-h) - 2f(c) + f(c+h)}{h^2} + 0(h^2). \tag{8.4}$$

Remark. From the above finite difference formulas, it seems that the approximation would become more and more accurate as $h \to 0$. This observation is true, however, only for exact arithmetic. In actually computation, there is a lower bound on h beyond which no improvement on accuracy should be expected. To understand this phenomenon, consider the central finite difference (8.2). Due to roundoff errors, we know $f(c+h) = \hat{f}(c+h) + E^+$ and $f(c-h) = \hat{f}(c-h) + E^-$ where $\hat{f}$ represents the floating point value of f. According to the formula, we are calculating $\hat{f}'(c) = \frac{\hat{f}(c+h)-\hat{f}(c-h)}{2h}$. Thus

$$f'(c) - \hat{f}'(c) = \frac{E^+ - E^-}{2h} + 0(h^2). \tag{8.5}$$

The second term in (8.5) is stable and converges to zero as $h \to 0$. But the first term becomes unbounded as $h \to 0$, since the numerator $E^+ - E^-$ is approximately equal to the machine accuracy and is bounded away from zero. Obviously using double precision in calculation can help to delay this from happening too soon.

8.2 Richardson Extrapolation

The Richardson extrapolation technique is often used to improve the accuracy from a set of already computed approximate solutions. The method works for both numerical differentiation and numerical integration. The idea is as follows:

Let q denote the true quantity needed. Let $N(q)$ denote the approximation to q by a specific numerical scheme. Usually these quantities are related by the equation:

$$N(q) = q + ch^m + 0(h^n) \tag{8.6}$$

where h is the stepsize used in the numerical scheme and $n > m$. Suppose we have already used, respectively, two different stepsizes $h = h_1$ and $h = h_2$ ($h_1 > h_2$) to obtain $N(q)_1$ and $N(q)_2$. Then

$$N(q)_1 = q + ch_1^m + 0(h_1^n), \tag{8.7}$$

$$N(q)_2 = q + ch_2^m + 0(h_2^n). \tag{8.8}$$

Let $k := \frac{h_1}{h_2}$. Then it is easy to see that

$$k^m N(q)_2 - N(q)_1 = (k^m - 1)q + 0(h_2^n). \tag{8.9}$$

Thus

$$M(q) := \frac{k^m N(q)_2 - N(q)_1}{k^m - 1} = q + 0(h_2^n) \tag{8.10}$$

is a higher order approximation to q.

8.3 Newton-Cotes Quadrature

Definition 8.3.1 *Given a function $f(x)$ defined on $[a, b]$, a formula of the form*

$$Q_n(f) := \sum_{i=1}^{n} \alpha_i f(x_i) \tag{8.11}$$

with $\alpha_i \in R$ and $x_i \in [a,b]$ is called a quadrature rule for the integral $I(f) := \int_a^b f(x)dx$. The points x_i are called the quadrature points (abscissas) and the values α_i are called the quadrature coefficients (weights). We also define the quadrature error $E_n(f) := I(f) - Q_n(f)$.

Definition 8.3.2 *A quadrature rule is said to have degree of precision m if $E_n(x^k) = 0$ for $k = 0, \ldots, m$ and $E_n(x^{m+1}) \neq 0$.*

Remark. If a quadrature rule has degree of precision m, then $E_n(p_k) = 0$ for all polynomials $p_k(x)$ of degree $\leq m$.
Examples.(1) (Trapezoidal Rule) Suppose we approximate $f(x)$ over $[a,b]$ by a segment joining points $(a, f(a))$ and $(b, f(b))$. Then

$$I(f) \approx Q_2(f) = \frac{b-a}{2}[f(a) + f(b)]. \tag{8.12}$$

Since $f(x) - p_1(x) = (x-a)(x-b)f[a,b,x]$, it follows that

$$E_2(f) = \int_a^b (x-a)(x-b)f[a,b,x]dx. \tag{8.13}$$

Observe that $(x-a)(s-b)$ does not change sign in $[a,b]$. By the mean value theorem, i.e. $\int_a^b f(x)g(x)dx = f(\xi)\int_a^b g(x)dx$ for some $\xi \in [a,b]$ if $g(x)$ is of one sign over $[a,b]$, we conclude that

$$\begin{aligned} E_2(f) &= f[a,b,\xi]\int_a^b (x-a)(x-b)dx \\ &= \frac{f^{(2)}(\eta)}{2}\frac{(b-a)^3}{6} = -\frac{f^{(2)}(\eta)}{12}(b-a)^3. \end{aligned} \tag{8.14}$$

(2) (Simpson's Rule) Suppose we approximate $f(x)$ by a quadratic polynomial $p_2(x)$ that interpolates $f(a), f\left(\frac{a+b}{2}\right)$ and $f(b)$. Then one can show that

$$Q_3(f) = \frac{b-a}{6}[f(a) + 4f(\frac{a+b}{2}) + f(b)]. \tag{8.15}$$

The error obviously is given by

$$E_3(f) = \int_a^b f[a,b,\frac{a+b}{2},x]\omega(x)dx \tag{8.16}$$

with $\omega(x) := (x-a)(x-b)(x-\frac{a+b}{2})$. The function $\omega(x)$ changes sign as x crosses $\frac{a+b}{2}$. So we have to analyze $E_3(x)$ by a different approach. Let $\Omega(x) := \int_a^x \omega(t)dt$. Then $\Omega'(x) = \omega(x)$. Thus by integration by parts, we have $E_3(f) = f[a,b,\frac{a+b}{2},x]\Omega(x)|_a^b - |_a^b f[a,b,\frac{a+b}{2},x,x]\Omega(x)dx$. Observe that $\Omega(a) = \Omega(b) = 0$. Observe also that $\Omega(x) > 0$ for all $x \in (a,b)$. Thus now we may apply the mean value theorem to conclude that

$$\begin{aligned} E_3(f) &= -\int_a^b f[a,b,\frac{a+b}{2},x,x]\Omega(x)dx = -f[a,b,\frac{a+b}{2},\xi,\xi]\int_a^b \Omega(x)dx \\ &= -\frac{f^{(4)}(\eta)}{4!}\frac{4}{15}\left(\frac{b-a}{2}\right)^5 = -\frac{f^{(4)}(\eta)}{90}\left(\frac{b-a}{2}\right)^5. \end{aligned} \tag{8.17}$$

Remark. The degree of precision for Simpson's rule is 3 rather than 2.

For a general integer $n > 1$, define $h := \frac{b-a}{n-1}, x_i := a + (i-1)h, i = 1, \ldots, n$. Let $p_{n-1}(x)$ be the Lagrangian interpolation polynomial of $f(x)$ at nodes $x_i, i = 1, \ldots, n$. Then we may write

$$f(x) = \sum_{i=1}^{n} f(x_i)\ell_i(x) + f[x_1, \ldots, x_n, x]\prod_{i=1}^{n}(x - x_i). \tag{8.18}$$

Thus we obtain a quadrature formula

$$I(f) = \sum_{i=1}^{n} \alpha_i f(x_i) + E_n(f) \tag{8.19}$$

with quadrature coefficients

$$\alpha_i := \int_a^b \ell_i(x)dx \tag{8.20}$$

and error

$$E_n(f) = \int_a^b f[x_1, \ldots, x_n, x]\prod_{i=1}^{n}(x - x_i)dx. \tag{8.21}$$

In general, the function $\omega_n(x) := \prod_{i=1}^{n}(x - x_i)$ changes sign in the interval $[a, b]$. But it can be proved that

Theorem 8.3.1 *(1) If n is odd and $f \in C^{n+1}$, then*

$$E_n(f) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\int_a^b x\omega_n(x)dx. \tag{8.22}$$

(2) If n is even and $f \in C^n$, then

$$E_n(f) = \frac{f^{(n)}(\xi)}{n!}\int_a^b \omega_n(x)dx. \tag{8.23}$$

(pf): This is a homework problem.

Definition 8.3.3 *The quadrature (8.19) obtained above is called a closed Newton-Cotes formula.*

Remark. Consider the Runge's function $f(x) = \frac{1}{1+x^2}$ defined over $[-5,5]$. We recall the fact that the interpolating polynomial using equally spaced nodes will not yield good convergence as $n \to \infty$. Consequently, we should not expect that the closed Newton-Cotes formula will yield accurate results for the integral. For instance, $I(f) = \int_{-4}^{4} \frac{1}{1+x^2}dx = 2\tan^{-1} 4 \approx 2.6516$. But the closed Newton-Cotes formula yields

n	3	5	7	9	11
$Q_n(f)$	5.4902	2.2776	3.3288	1.9411	3.5956

For this reason, we seldom use the Newton-Cotes formula for $n > 5$ in practice. Instead, we limit $n \leq 5$ and the so called composited rules.

Definition 8.3.4 *In calculating the integral of a function $f(x)$ over an interval $[a,b]$, we first divide $[a,b]$ into a number of subintervals, and then apply the Newton-Cotes formula with lower n to each subinterval, and then add the results. Such a method is called a Composited Newton-Cotes formula.*

Example. Suppose the interval $[a,b]$ is divided into an even number, say $2m$, of subintervals. Let $h = \frac{b-a}{2m}, x_i = a + ih, i = 0, 1, \ldots, 2m$. Then the composite simpson's rule takes the form

$$\begin{aligned}\int_a^b f(x)dx &= \frac{h}{3}\left\{f(a) + 2\sum_{i=1}^{m-1} f(x_{2i}) + 4\sum_{i=0}^{m-1} f(x_{2i+1}) + f(b)\right\} \\ &- \frac{(b-a)}{180}h^4 f^{(4)}(\xi). \end{aligned} \tag{8.24}$$

Remark. Suppose $f(x_i) = y_i + \epsilon_i$ where y_i is the floating point number approximation to $f(x_i)$ and ϵ_i is the roundoff error. Upon substituting these values into (8.24), we obtain

$$\begin{aligned}\int_a^b f(x)dx &= \frac{h}{3}\left\{y_0 + 2\sum_{i=1}^{m-1} y_{2i} + 4\sum_{i=0}^{m-1} y_{2i+1} + y_{2m}\right\} \\ &+ \frac{h}{3}\left\{\epsilon_0 + 2\sum_{i=1}^{m-1} \epsilon_{2i} + f\sum_{i=0}^{m-1} \epsilon_{2i+1} + \epsilon_{2m}\right\}. \end{aligned} \tag{8.25}$$

Suppose $|\epsilon_i| \leq \epsilon$. Then the error due to roundoff is bounded by $\frac{h}{3}6m\epsilon = (b-a)\epsilon$. Thus, unlike the process of numerical differentiation, numerical integration using composite rule is a stable process in the sense that the error due to roundoff is independent of the stepsize h.

8.4 Gaussian Quadrature

The Newton-Cotes formula for the integral $I(f) = \int_a^b f(x)dx$ is based on the integration of the polynomial $p(x)$ that interpolates $f(x)$ at a set of equally spaced nodes in $[a, b]$. Gaussian quadrature results from a different approach in which both the abscissas x_i and weights α_i are to be determined so that the quadrature

$$Q_n(f) = \sum_{i=1}^{n} \alpha_i f(x_i) \tag{8.26}$$

has a maximal degree of precision. Since there are $2n$ unknowns in (8.26), the requirements

$$E_n(x^k) = 0, k = 0, 1, \ldots, 2n-1 \tag{8.27}$$

supply $2n$ equations. Thus it is expected that the maximal degree of precision is $\geq 2n-1$. The condition (8.27) is equivalent to

$$\sum_{i=1}^{n} \alpha_i x_i^k = \frac{b^{k+1} - a^{k+1}}{k+1}, k = 0, 1, \ldots, 2n-1 \tag{8.28}$$

which is a nonlinear system. It is not clear whether (8.28) always has a solution for arbitrary a and b. Neither is it clear whether the solution of (8.28) is real-valued or not.

Theorem 8.4.1 *A quadrature formula using n distinct abscissas results from the integration of an interpolation polynomial if and only if the quadrature has degree of precision $\geq n-1$.*

(pf): ($\Longrightarrow$) This follows from Theorem 8.3.1.

($\Longleftarrow$) Suppose the quadrature $\sum_{i=1}^{n} \alpha_i f(x_i)$ has degree of precision $\geq n-1$. Then $\sum_{i=1}^{n} \alpha_i x_i^k = \frac{b^{k+1} - a^{k+1}}{k+1}$ for $k = 0, \ldots, n-1$. We may rewrite this system of equations as

$$\begin{bmatrix} 1 & 1 \\ x_1 & x_n \\ \\ x_1^{n-1}, \ldots & x_n^{n-1} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \\ \\ a_n \end{bmatrix} = \begin{bmatrix} b-a \\ \\ \\ \frac{b^n - a^n}{n} \end{bmatrix}. \tag{8.29}$$

The coefficient matrix is the von de Morde matrix. Thus system (8.29) has a unique solution for (α_i). On the other hand, we can construct an interpolating polynomial using the same nodes $\{x_i\}$. This polynomial results in a quadrature formula $\sum_{i=1}^{n} \beta_i f(x_i)$ which has degree of precision $\geq n-1$. By setting $E_n(x^k) = 0$ for $k = 0, \ldots, n-1$, we end up with the same linear system (8.29). By uniqueness, it must be that $\alpha_i = \beta_i$. $\oplus$

By Theorem 8.4.1, the gaussian quadrature may be thought of as the integration of ascertain polynomial that interpolates $f(x)$ at a certain set of nodes

$x_1, \ldots, x_n$. In this sense, we still find

$$E_n(f) = \int_a^b f[x_1, \ldots, x_n, x] \prod_{i=1}^{n} (x - x_i) dx. \tag{8.30}$$

Not only $E_n(x^k) = 0$ for $k = 0, \ldots, n-1$, but we further would like to require $E_n(x^k) = 0$ for $k = n, \ldots, n+\nu$, and for ν as large as possible. There are two approaches to accomplish this goal:

Lemma 8.4.1 *If $f(x) = x^{n+\nu}, \nu \geq 0$, then the n-th divided difference $f[x_1, \ldots, x_n, x]$ is a polynomial of degree at most ν.*

(pf): When $n = 1$, we find $f[x_1, x] = \frac{f(x_1)-f(x)}{x_1-x} = \frac{x_1^{1+\nu}-x^{1+\nu}}{x_1-x}$ is obviously a polynomial of degree ν. Suppose the assertion is true for $n = k$. Consider $f(x) = x^{k+1+\nu}$. Then $f[x_2, \ldots, x_{k+1}, x]$, by induction hypothesis, is a polynomial of degree at most $\nu + 1$. Observe that $f[x_1, \ldots, x_{k+1}, x] = \frac{f[x_1, \ldots, x_{k+1} - f[x_2, \ldots, x_{k+1}, x]}{x_1 - x}$. Note that the numerator has a zero at $x = x_1$. Thus $f[x_1, \ldots, x_{k+1}, x]$ is a polynomial of degree of most ν. The assertion now follows from the induction. $\oplus$

From (8.30) and Lemma 8.4.1, we see that $E_n(f) = 0$ for $f(x) = x^n, \ldots, x^{n+\nu}$ if and only if $\int_a^b x^k \prod_{i+1}^{n} (x - x_i) dx = 0$ holds for $k = 0, 1, \ldots, \nu$. Thus we are seeking $\{x_i\}$ so that $\omega_n(x) := \prod_{i=1}^{n} (x - x_i)$ is perpendicular to functions $1, x, \ldots, x^\nu$. Since $\omega_n^{(x)}$ is a polynomial of degree n, we cannot have $\nu \geq n$; otherwise, the polynomial $\omega_n(x)$ would be perpendicular to itself. Is it then possible to have $\nu = n - 1$? The answer is positive.

Lemma 8.4.2 *From the basic polynomials $1, x, x^2, \ldots$ and the inner product $< f, g >:= \int_a^b f(x)g(x)dx$, we can generate a new basis of polynomials $\{\phi_k(x)\}$ such that ϕ_k is of degree k, and $< \phi_i, \phi_h >= 0$ whenever $i \neq j$. The ϕ_k's are unique up to constant multipliers.*

(pf): The assertion follows from the standard Gram-Schmidt orthogonalization process. $\oplus$

From the above discussion, we conclude that we may select the quadrature coefficients $\{\alpha_i\}$ and the nodes $\{x_i\}$ in the formula (8.26) such that the quadrature has degree of precision $2n - 1$. Such a formula is interpolating the function $f(x)$ at x_i which are zeros of the n-th orthogonal polynomial, that is, $\omega_n(x) = c\phi_n(x)$. In this case, $\alpha_i = \int_a^b \ell_i(x)dx = \int_a^b \prod_{j \neq i}^{n} \frac{x - x_j}{x_i - x_j} dx = \frac{1}{\phi_n(x_i)} \int_a^b \frac{\phi_n(x)}{x - x_i} dx$. This formula is called the gaussian quadrature formula.

Remark. Without loss of generality, we may assume $[a,b]=[-1,1]$. In this case, the orthogonal polynomial are known as the Legendre's polynomials and are given by:

$$\begin{aligned} P_0(x) &= 1, && (8.31)\\ P_1(x) &= x, && (8.32)\\ P_2(x) &= \frac{1}{2}(3x^2-1), && (8.33)\\ P_k(x) &= \frac{1}{2^k k!}\frac{d^k}{dx^k}(x^2-1)^k. && (8.34) \end{aligned}$$

The resulting quadrature is known as the Gauss-Legendre quadrature formula.

Theorem 8.4.2 *All the n zeros of the orthogonal polynomial $\phi_n(x)$ are real-valued, distinct, and contained in (a,b).*

(pf): Let $x_1,\ldots,x_m \in (a,b)$ denote all the distinct, real zeros of $\phi_n(x)$ with odd multiplicity. Assume $m<n$. Consider the integral $\int_a^b (x-x_1)\ldots(x-x_m)\phi_n(x)dx$. Note that the integrand does not change sign over $[a,b]$ and is not identically zero. Thus the integral is positive. On the other hand, observe that $(x-x_1)\ldots(x-x_m)$ is a polynomial of degree $m<n$. By orthogonality of $\phi_n(x)$, the integral should be zero. This is a contradiction. Thus it must be that $m=n$, and the multiplicity is 1.

We now consider another approach to the Gaussian quadrature. Recall the Hermite interpolation formula for $f(x)$ (Example 1 in Section 7.3):

$$\begin{aligned} f(x) &= \sum_{i=1}^{n} h_i(x)f(a_i) + \sum_{i=1}^{n} g_i(x)f'(a_i)\\ &+ \frac{\omega_n^2(x)}{(2n)!}f^{(2n)}(\xi) && (8.35) \end{aligned}$$

where

$$\begin{aligned} h_i(x) &= [1-2(x-a_i)\ell_i'(a_i)]\ell_i^2(x) && (8.36)\\ g_i(x) &= (x-a_i)\ell_i^2(x) && (8.37) \end{aligned}$$

and $\ell_i(x)$ is the Lagrangian interpolation polynomial

$$\ell_i(x) = \prod_{\substack{j=1\\ j\neq i}}^{n} \frac{x-a_j}{a_i-a_j} = \frac{\omega_n(x)}{(x-a_i)\omega_n'(a_i)} \qquad (8.38)$$

and

$$\omega_n(x) = \prod_{i=1}^{n}(x-a_i). \qquad (8.39)$$

Remark. Recall that

$$\ell_i(a_k) = \delta_{ik}, i, k = 1, \ldots, n. \tag{8.40}$$

and the properties

$$\begin{aligned} h_i(a_k) &= g_i'(a_k) = \delta_{ik} & (8.41)\\ g_i(a_k) &= h_i'(a_k) = 0, i, k = 1, \ldots, n. & (8.42) \end{aligned}$$

Remark. Since the Hermite interpolation polynomial interpolates f and f' at n nodes, we know that the Hermite polynomial is exactly the same f if f is a polynomial of degree $2n-1$ or less.

Integrating (8.35) over the interval $[a, b]$, we get

$$\int_a^b f(x)dx = \sum_{i=1}^n \alpha_i f(a_i) + \sum_{i=1}^n \beta_i f'(a_i) + E_n(f) \tag{8.43}$$

where

$$\begin{aligned} \alpha_i &= \int_a^b h_i(x)dx & (8.44)\\ \beta_i &= \int_a^b g_i(x)dx & (8.45)\\ E_n(f) &= \int_a^b \frac{\omega_n^2(x)}{(2n)!} f^{(2n)}(\xi)dx. & (8.46) \end{aligned}$$

Note $E_n(f)$ is automatically zero if $f(x)$ is a polynomial of degree $2n-1$ or less. If we can choose the abscissas so that $\beta_j = 0, j = 1, \ldots, n$, then (8.43) will have the form (8.26) with the desired degree of precision. That is,

$$\beta_j = 0, j = 1, \ldots, n, \tag{8.47}$$

is a sufficient condition for the quadrature (8.26) to have degree of precision $2n-1$. The condition (8.47) is also necessary. This can be seen from letting $f(x) = g_j(x)$ in (8.26). Since $g_j(x)$ is a polynomial of degree $2n-1, E_n(g_j) = 0$. But also $\beta_j = I(g_j) = Q_n(g_j) = \sum_{i=1}^n \alpha_i g_j(x_i) = 0$ because of the property (8.41) and (8.42).

Using (8.37) and (8.45), we have

$$\beta_j = \int_a^b (x - a_j)\ell_j^2(x)dx = \int_a^b \omega_n(x)\frac{\ell_j(x)}{\omega_n'(a_j)}dx. \tag{8.48}$$

Since $\omega_n(x)$ is a polynomial of degree n and $\ell_j(x)$ is a polynomial of degree $n-1$, a sufficient condition for $\beta_j = 0, j = 1, \ldots, n$, is that $\omega_n(x)$ be orthogonal to all polynomials of degree $n-1$ or less over $[a, b]$. It can be proved that this condition is also necessary. This is done by letting $f(x) = \omega_n(x)u_{n-1}(x)$ in (8.26) where $u_{n-1}(x)$ is an arbitrary polynomial of degree $n-1$ or less. Since

(8.26) is exact for polynomials of degree $2n-1$ or less we have $I(\omega_n u_{n-1}) = \sum_{i=1}^{n} \alpha_i \omega_n(a_i) u_{n-1}(a_i) = 0$, that is,

$$\omega_n \perp u_{n-1}. \tag{8.49}$$

Remark. By now we have reached the same conclusion as the other approach on the property of the function $\omega_n(x)$. Assume $[a,b]=[1,-1]$. Then

$$\omega_n(x) = \frac{2^n (n!)^2}{(2n)!} P_n(x) \tag{8.50}$$

where $P_n(x)$ is the well-known Legendre polynomial defined by

$$P_0(x) = 1 \tag{8.51}$$
$$P_1(x) = x \tag{8.52}$$
$$P_{k+1}(x) = \frac{2k+1}{k+1} x P_k(x) - \frac{k}{k+1} P_{k-1}(x). \tag{8.53}$$

We have seen from Theorem (8.4.2) that the zeros of the Legendre polynomial of any degree are real, so this settles the question of the existence of real abscissa. To find the weights we use (8.37) and (8.45) to get

$$\begin{aligned} \alpha_j &= \int_{-1}^{1} h_j(x)dx = \int_{-1}^{1} [1 - 2(x-a_j)\ell_j'(a_j)]\ell_j^2(x)dx \\ &= \int_{-1}^{1} \ell_j^2(x)dx - 2\ell_j'(a_j) \int_{-1}^{1} (x-a_j)\ell_j^2(x)dx \\ &= \int_{-1}^{1} \ell_j^2(x)dx \end{aligned} \tag{8.54}$$

since the second integral, which by definition is β_j, is zero. From (8.54) it is obvious that the wieghts are all positive. By considering (8.26) with $f(x) = \ell_j(x)$, which is a ploynomial of degree $n-1$, we have

$$\int_{-1}^{1} \ell_j(x)dx = \sum_{i=1}^{n} \alpha_i \ell_j(a_i) = \alpha_j \tag{8.55}$$

since $\ell_j(a_i) = \delta_{ji}$. Together (8.54) and (8.55) imply that

$$\alpha_j = \int_{-1}^{1} \ell_j^2(x)dx = \int_{-1}^{1} \ell_j(x)dx. \tag{8.56}$$

The following talbe shows the abscissas and weights for values of n of practical interest.

n	Abscissas x_j	Weights α_j
2	$\pm 1/\sqrt{3}$	1
3	$\pm\sqrt{0.6}$	5/9
	0	8/9
4	± 0.8611363116	0.3478548451
	± 0.3399810436	0.6521451549
5	± 0.9061798459	0.2369268850
	± 0.5384693101	0.4786286705
	0	0.5688888889
6	± 0.9324695142	0.1713244924
	± 0.6612093865	0.3607615730
	± 0.2386191861	0.4679139346

To use Gauss quadrature to integrate $f(x)$ over an arbitrary interval $[a, b]$, we simply map the ξ-interval $[-1, 1]$ into the x-interval $[a, b]$ using the linear transformation

$$x = a + \frac{b-a}{2}(\xi + 1), dx = \frac{b-a}{2} d\xi. \tag{8.57}$$

Making this substitution in (8.26) gives

$$\begin{aligned} \int_a^b f(x)dx &= \int_{-1}^1 f(a + \frac{b-a}{2}(\xi+1))\frac{b-a}{2} d\xi & (8.58) \\ &= \frac{b-a}{2}\int_{-1}^1 f(a + \frac{b-a}{2}(\xi+1)) d\xi & (8.59) \\ &\approx \frac{b-a}{2}\sum_{i=1}^n \alpha_i f(x_i) & (8.60) \end{aligned}$$

where α_j are the tabulated gaussian weights associated with the tabulated gaussian abscissa a_j in $[-1, 1]$, and x_j is obtained from a_j as follows:

$$x_j = a + \frac{b-a}{2}(a_j + 1), j = 1, \ldots, n. \tag{8.61}$$

8.5 Other gaussian Quadratures

Depending on the applications, sometimes it is necessary to integrate a function $f(x)$ with respect to a specified weight function $w(x)$, i.e.,

$$I_w(f) := \int_a^b w(x)f(x)dx \tag{8.62}$$

where $w(x) \geq 0$ on $[a, b]$. In such a case, we consider a quadrature rule of the form

$$Q_w(f) := \sum_{i=1}^{n} \alpha_i f(x_i). \tag{8.63}$$

Note that the weight function $w(x)$ does not appear on the right hand side of (8.63). Using the same idea as discussed in the preceding section, it can be proved that a sufficient and necessary condition for $Q_w(f)$ to have as high the degree of precision as possible is that the nodes x_i are the zeros of an orthogonal polynomial with respect to $w(x)$. That is, if $\omega_n(x) := \prod_{i=1}^{n}(x - x_i)$, then

$$\int_a^b w(x) u_{n-1}(x) \omega_n(x) dx = 0 \tag{8.64}$$

for every polynomial $u_{n-1}(x)$ of degree $\geq n - 1$. In this case, the quadrature coefficients are

$$\alpha_i := \int_a^b w(x) \ell_i(x) dx \tag{8.65}$$

and the quadrature error is

$$E_w(f) = \frac{f^{(2)}(\xi)}{(2n)!} \int_a^b w(x) \omega_n^2(x) dx. \tag{8.66}$$

Without repeating the arguments, we simply summarize below some of the well known Gaussian formulas:

Weight function $w(x)$	Interval $[a, b]$	Abscissas are zeros of	Name of the special orthogonal polynomial
1	$[-1, 1]$	$P_n(x)$	Legendre
e^{-x}	$[0, \infty]$	$L_n(x)$	Laguerre
e^{-x^2}	$[-\infty, \infty]$	$H_n(x)$	Hermite
$(1-x)^\alpha (1+x)^\beta$	$[-1, 1]$	$J_n(x; \alpha, \beta)$	Jacobi
$\frac{1}{(1-x^2)^{1/2}}$	$[-1, 1]$	$T_n(x) = \cos(n \cos^{-1} x)$	Chebyshev, 1-st kind
$(1-x^2)^{1/2}$	$[-1, 1]$	$S_n(x) = \frac{\sin((n+1)\cos^{-1} x}{\sin(cos^{-1} x)}$	Chebyshev, 2-nd king
$\frac{1}{\sqrt{x}}$	$[0, 1]$	$P_{2n}(\sqrt{x}$	
$\sqrt{x}$	$[0, 1]$	$\frac{1}{\sqrt{s}} P_{2n+1}(\sqrt{x})$	
$(\frac{x}{1-x})^{1/2}$	$[0, 1]$	$\frac{1}{\sqrt{x}} T_{2n+1}(\sqrt{x})$	

8.6 Adaptive Integration

Recall the equally-spaced composite Simpson's rule

$$\begin{aligned}\int_a^b f(x)dx &= \frac{h}{3}\{f(x_0) + 2\sum_{i=1}^{m-1} f(x_{2i}) \\ &\quad +4\sum_{i=0}^{m-1} f(x_{2i+1}) + f(x_{2m})\} - \frac{(b-a)}{180}h^4 f^{(4)}(\xi). \quad (8.67)\end{aligned}$$

Obviously, if $f^{(4)}(x)$ various greatly in magnitude, then the error term in (8.67) might not be reasonable. In practice, we should not introduce more than what is necessarily many nodes to save the overhead. But near points where $f(x)$ behaves badly we should place denser nodes to maintain the accuracy. For these reasons, we introduce an adaptive integration method which performs a local error estimation and introduce nodes according to the behavior of the integrand.

Let $a = a_0 < a_1 < \ldots < a_n = b$ be a partition of $[a, b]$ where

$$h_i := a_{i+1} - a_i \quad (8.68)$$

generally are of different lengths but are of the form $\frac{b-a}{2^r}$. Such an interval is said to be of level r. Consider the two quadrature rules over the interval $[a_i, a_{i+1}]$:

$$\begin{aligned} R_2[a_i, a_{i+1}](f) &= \frac{h_i}{12}\{f(a_i) + 4f(a_i + \frac{h_i}{4}) \\ &+ 2f(a_i + \frac{h_i}{2}) + 4f(a_i + \frac{3h_i}{4}) + f(a_{i+1})\} \quad (8.69)\end{aligned}$$

$$R_1[a_i, a_{i+1}](f) = \frac{h_i}{6}\{f(a_i) + 4f(a_i + \frac{h_i}{2}) + f(a_{i+1})\} \quad (8.70)$$

Suppose that the nodes $a_0, \ldots, a_i$ have already been determined so that

$$\int_a^{a_i} f(x)dx \approx \sum_{j=1}^{i} R_2[a_{j-1}, a_j](f) \quad (8.71)$$

has already been accepted as an approximation. We want to consider the next stepsize h at the level r. Observe from (8.67) that

$$\begin{aligned} &\int_\alpha^{\alpha+h} f(x)dx - R_1[\alpha, \alpha+h](f) = -\frac{\hat{h}^5}{90} f^{(4)}(\xi) \\ &= \frac{\hat{h}^5}{90} f^{(4)}(\alpha + \frac{h}{2}) + O(h^6), \quad (8.72) \\ &\int_\alpha^{\alpha+h} f(x)dx - R_2[\alpha, \alpha+h](f) = -\frac{\hat{h}^5}{1440} f^{(4)}(\xi) \\ &= -\frac{\hat{h}^5}{1440} f^{(4)}(\alpha + \frac{h}{2}) + 0(h^6) \quad (8.73)\end{aligned}$$

with $\hat{h} := \frac{h}{2}$. Thus

$$R_2[\alpha, \alpha + h](f) - R_1[\alpha, \alpha + \frac{h}{2}](f) \approx \frac{15\hat{h}^5}{1440} f^{(4)}(\alpha + h) \tag{8.74}$$

and

$$\int_{\alpha}^{\alpha+h} f(x)dx - R_2[\alpha, \alpha + h](f) \approx \frac{1}{15}(R_2 - R_1). \tag{8.75}$$

In order that $| \int_{a_i}^{a_i+h} f(x)dx - R_2[a_i, a_i + h](f)| < \frac{\epsilon}{2^r}$, we check to see if

$$|R_2[a_i, a_i + h](f) - R_1[a_i, a_i + h](f)| < \frac{15\epsilon}{2^r}. \tag{8.76}$$

If (8.72) holds, we define $a_{i+1} := a_i + h$, add $R_2[a_i, a_{i+1}](f)$ to the right hand side of (8.66) to obtain an approximation of $\int_a^{a_{i+1}} f(x)dx$, and go on to the next subinterval. If (8.76) does not hold, we then consider the intervals $[a_i, a_i + \frac{h}{2}]$ and $[a_i + \frac{h}{2}, a_i + h]$ at the level $r + 1$. All the previously computed values should be saved for future use. The integration is stopped when a subinterval $[a_{n-1}, b]$ converges. A flowchart of the adaptive integration method is as follows:
Remark. The flowchart of adoptive integration method.