6 Numerical Integration

6.1 Basic Concepts

In this chapter we are going to explore various ways for approximating the integral of a function over a given domain. There are various reasons as of why such approximations can be useful. First, not every function can be analytically integrated. Second, even if a closed integration formula exists, it might still not be the most efficient way of calculating the integral. In addition, it can happen that we need to integrate an unknown function, in which only some samples of the function are known.

In order to gain some insight on numerical integration, it is natural to review Riemann integration, a framework that can be viewed as an approach for approximating integrals. We assume that $f(x)$ is a bounded function defined on $[a,b]$ and that $\{x_0,\ldots,x_n\}$ is a partition (P) of $[a,b]$. For each i we let

$$M_i(f) = \sup_{x\in[x_{i-1},x_i]} f(x),$$

and

$$m_i(f) = \inf_{x\in[x_{i-1},x_i]} f(x),$$

Letting $\Delta x_i = x_i - x_{i-1}$, **the upper (Darboux) sum** of $f(x)$ with respect to the partition P is defined as

$$U(f,P) = \sum_{i=1}^{n} M_i \Delta x_i, \tag{6.1}$$

while **the lower (Darboux) sum** of $f(x)$ with respect to the partition P is defined as

$$L(f,P) = \sum_{i=1}^{n} m_i \Delta x_i. \tag{6.2}$$

The upper integral of $f(x)$ on $[a,b]$ is defined as

$$U(f) = \inf(U(f,P)),$$

and **the lower integral** of $f(x)$ is defined as

$$L(f) = \sup(L(f,P)),$$

where both the infimum and the supremum are taken over all possible partitions, P, of the interval $[a,b]$. If the upper and lower integral of $f(x)$ are equal to each other, their common value is denoted by $\int_a^b f(x)dx$ and is referred to as **the Riemann integral** of $f(x)$.

For the purpose of the present discussion we can think of the upper and lower Darboux sums (6.1), (6.2), as two approximations of the integral (assuming that the function is indeed integrable). Of course, these sums are not defined in the most convenient way for an approximation algorithm. This is because we need to find the extrema of the function in every subinterval. Finding the extrema of the function, may be a complicated task on its own, which we would like to avoid.

A simpler approach for approximating the value of $\int_a^b f(x)dx$ would be to compute the product of the value of the function at one of the end-points of the interval by the length of the interval. In case we choose the end-point where the function is evaluated to be $x = a$, we obtain

$$\int_a^b f(x)dx \approx f(a)(b-a). \tag{6.3}$$

This approximation (6.3) is called **the rectangular method** (see Figure 6.1). Numerical integration formulas are also referred to as **integration rules** or **quadratures**, and hence we can refer to (6.3) as the rectangular rule or the rectangular quadrature. The points $x_0, \ldots x_n$ that are used in the quadrature formula are called **quadrature points**.

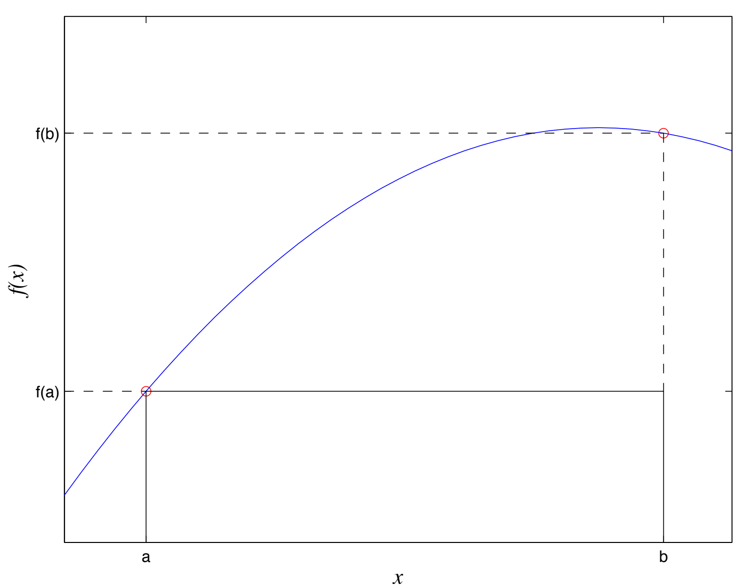

Figure 6.1: A rectangular quadrature

A variation on the rectangular rule is **the midpoint rule**. Similarly to the rectangular rule, we approximate the value of the integral $\int_a^b f(x)dx$ by multiplying the length of the interval by the value of the function at one point. Only this time, we replace the value of the function at an endpoint, by the value of the function at the center point

$\frac{1}{2}(a+b)$, i.e.,

$$\int_a^b f(x)dx \approx (b-a)f\left(\frac{a+b}{2}\right). \tag{6.4}$$

(see also Fig 6.2). As we shall see below, the midpoint quadrature (6.4) is a more accurate quadrature than the rectangular rule (6.3).

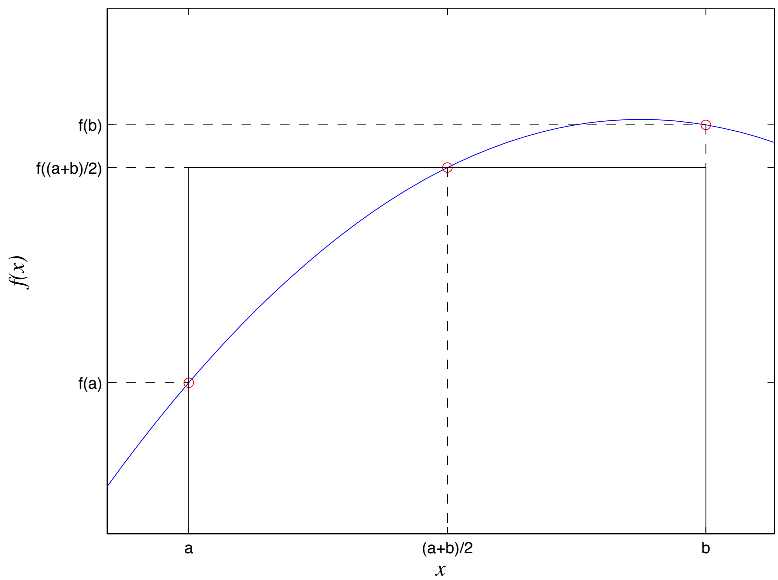

Figure 6.2: A midpoint quadrature

In order to compute the quadrature error for the midpoint rule (6.4), we consider the primitive function $F(x)$,

$$F(x) = \int_a^x f(s)ds,$$

and expand

$$\begin{aligned} \int_a^{a+h} f(s)ds = F(a+h) &= F(a) + hF'(a) + \frac{h^2}{2}F''(a) + \frac{h^3}{6}F'''(a) + O(h^4) \qquad (6.5) \\ &= hf(a) + \frac{h^2}{2}f'(a) + \frac{h^3}{6}f''(a) + O(h^4) \end{aligned}$$

If we let $b = a+h$, we have (expanding $f(a+h/2)$) for the quadrature error, E,

$$\begin{aligned} E = \int_a^{a+h} f(s)ds - hf\left(a+\frac{h}{2}\right) &= hf(a) + \frac{h^2}{2}f'(a) + \frac{h^3}{6}f''(a) + O(h^4) \\ &- h\left[f(a) + \frac{h}{2}f'(a) + \frac{h^2}{8}f''(a) + O(h^3)\right], \end{aligned}$$

which means that the error term is of order $O(h^3)$. Having an error of order h^3 does not mean that this is a third-order method. In our case, the parameter h equals to $b-a$. It is not a parameter that should be vied as a small value that goes to zero. It is fixed. The error of the midpoint method is of the order of $O((b-a)^3)$. Unfortunately, these calculations cannot directly provide us with an accurate estimate of the error. This is the case since when truncating two Taylor approximations, we are left with an error terms that are evaluated at two (generally different) intermediate points. Hence we cannot directly combine the error term $\frac{1}{6}h^3 f''(\xi_1)$ with $-\frac{1}{8}h^3 f''(\xi_2)$. This can still be done, but we have to use a better approach.

The main difficulty in evaluating the difference between the exact value, $\int_a^b f(x)dx$, and its midpoint rule approximation, $(b-a)f\left(\frac{a+b}{2}\right)$, is due to having an integral in one term and no integral in the second term. The approach will be to replace the midpoint approximation with an integral expression. Indeed, if we denote the midpoint by c, i.e.,

$$c = \frac{a+b}{2},$$

then the tangent line to $f(x)$ at $x = c$ is given by

$$P_1(x) = f(c) + f'(c)(x-c).$$

Clearly,

$$\int_a^b P_1(x)dx = (b-a)f(c),$$

and hence

$$\int_a^b f(x)dx - (b-a)f\left(\frac{a+b}{2}\right) = \int_a^b (f(x) - P_1(x))dx.$$

To estimate the difference between $f(x)$ and $P_1(x)$ we can expand $f(x)$ around $x = c$. Assuming that $x \in [a,b]$, we have

$$f(x) = f(c + (x-c)) = f(c) + f'(c)(x-c) + \frac{1}{2}f''(\xi)(x-c)^2, \qquad \xi \in (a,b).$$

Hence

$$\int_a^b (f(x) - P_1(x))dx = \int_a^b \frac{1}{2}f''(\xi_x)(x-c)^2 dx.$$

In view of the midvalue theorem for integrals, the last integral can be replaces by

$$\frac{1}{2}f''(\xi)\int_a^b (x-c)^2 dx = \frac{1}{24}(b-a)^3 f''(\xi), \qquad a < \xi < b. \tag{6.6}$$

Remark. Throughout this section we assumed that all functions we are interested in integrating are actually integrable in the domain of interest. We also assumed that they are bounded and that they are defined at every point, so that whenever we need to evaluate a function at a point, we can do it. We will go on and use these assumptions throughout the chapter.

6.2 Integration via Interpolation

One direct way of obtaining quadratures from given samples of a function is by integrating an interpolant. As always, our goal is to evaluate $I = \int_a^b f(x)dx$. We assume that the values of the function $f(x)$ are given at $n+1$ points: $x_0, \ldots, x_n \in [a, b]$. Note that we do not require the first point x_0 to be equal to a, and the same holds for the right side of the interval. Given the values $f(x_0), \ldots f(x_n)$, we can write the interpolating polynomial of degree $\leqslant n$, which in the Largenge form is

$$P_n(x) = \sum_{i=0}^{n} f(x_i) l_i(x),$$

with

$$l_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}, \qquad 0 \leqslant i \leqslant n.$$

The integral of $f(x)$ can then be approximated by the integral of $P_n(x)$, i.e.,

$$\int_a^b f(x)dx \approx \int_a^b P_n(x)dx = \sum_{i=0}^{n} f(x_i) \int_a^b l_i(x)dx = \sum_{i=0}^{n} A_i f(x_i). \tag{6.7}$$

The quadrature coefficients A_i in (6.7) are given by

$$A_i = \int_a^b l_i(x)dx. \tag{6.8}$$

Note that if we want to integrate several different functions, and use their values at the same points $(x_0, \ldots, x_n)$, the quadrature coefficients (6.8) should be computed only once, since they do not depend on the function that is being integrated. If we change the interpolation/integration points, then we must recompute the quadrature coefficients.

For equally spaced points, $x_0, \ldots, x_n$, a numerical integration formula of the form

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} A_i f(x_i), \tag{6.9}$$

is called a **Newton-Cotes formula**.

Example 6.1
We let $n = 1$ and consider two interpolation points which we set as

$$x_0 = a, \quad x_1 = b.$$

In this case

$$l_0(x) = \frac{b - x}{b - a}, \qquad l_1(x) = \frac{x - a}{b - a}.$$

Hence

$$A_0 = \int_a^b l_0(x) = \int_a^b \frac{b-x}{b-a}dx = \frac{b-a}{2}.$$

Similarly,

$$A_1 = \int_a^b l_1(x) = \int_a^b \frac{x-a}{b-a}dx = \frac{b-a}{2} = A_0.$$

The resulting quadrature is the so-called **trapezoidal rule**,

$$\int_a^b dx \approx \frac{b-a}{2}[f(a)+f(b)], \tag{6.10}$$

(see Figure 6.3).

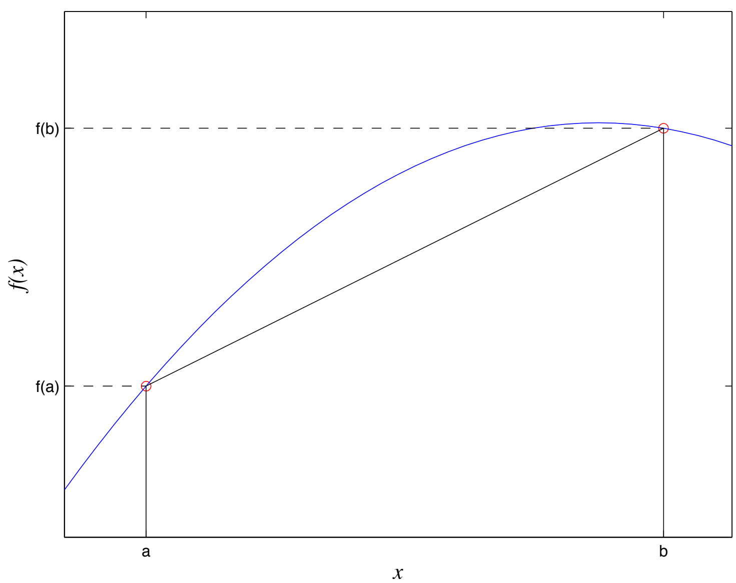

Figure 6.3: A trapezoidal quadrature

We can now use the interpolation error to compute the error in the quadrature (6.10). The interpolation error is

$$f(x) - P_1(x) = \frac{1}{2}f''(\xi_x)(x-a)(x-b), \qquad \xi_x \in (a,b).$$

We recall that according to the midvalue theorem for integrals, if $u(x)$ and $v(x)$ are continuous on $[a,b]$ and if $v \geqslant 0$, then there exists $\xi \in (a,b)$ such that

$$\int_a^b u(x)v(x)dx = u(\xi)\int_a^b v(x)dx.$$

Hence, the interpolation error is given by

$$E = \int_a^b \frac{1}{2} f''(\xi_x)(x-a)(x-b) = \frac{f''(\xi)}{2} \int_a^b (x-a)(x-b)dx = -\frac{f''(\xi)}{12}(b-a)^3, \quad (6.11)$$

with $\xi \in (a,b)$.

Remarks.

1. We note that the quadratures (6.7),(6.8), are exact for polynomials of degree $\leqslant n$. For if $p(x)$ is a polynomial of degree $\leqslant n$, it can be written as

$$p(x) = \sum_{i=0}^{n} p(x_i) l_i(x).$$

(Two polynomials of degree $\leqslant n$ that agree with each other at $n+1$ points must be identical). Hence

$$\int_a^b p(x)dx = \sum_{i=0}^{n} p(x_i) \int_a^b l_i(x)dx = \sum_{i=0}^{n} A_i p(x_i).$$

2. As of the opposite direction. Assume that the quadrature

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} A_i f(x_i),$$

is exact for all polynomials of degree $\leqslant n$. We know that

$$\deg(l_j(x)) = n,$$

and hence

$$\int_a^b l_j(x)dx = \sum_{i=0}^{n} A_i l_j(x_i) = \sum_{i=0}^{n} A_i \delta_{ij} = A_j.$$

This menas that the quadrature coefficients must be given by

$$A_j = \int_a^b l_j(x)dx.$$

6.3 Composite Integration Rules

In a composite quadrature, we divide the interval into subintervals and apply an integration rule to each subinterval. We demonstrate this idea with a couple of examples.

Example 6.2
Consider the points

$$a = x_0 < x_1 < \cdots < x_n = b.$$

The **composite trapezoidal rule** is obtained by applying the trapezoidal rule in each subinterval $[x_{i-1}, x_i]$, $i = 1, \ldots, n$, i.e.,

$$\int_a^b f(x)dx = \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} f(x)dx \approx \frac{1}{2} \sum_{i=1}^{n} (x_i - x_{i-1})[f(x_{i-1}) + f(x_i)], \tag{6.12}$$

(see Figure 6.4).

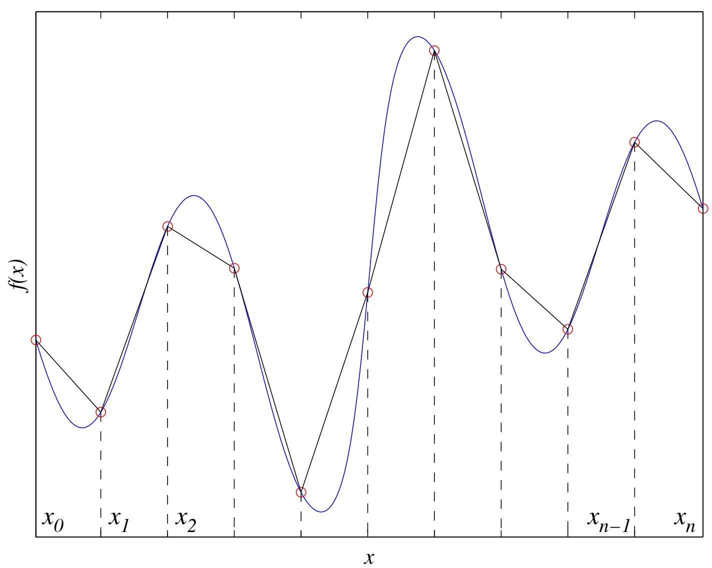

Figure 6.4: A composite trapezoidal rule

A particular case is when these points are uniformly spaced, i.e., when all intervals have an equal length. For example, if

$$x_i = a + ih,$$

where

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

then

$$\int_a^b f(x)dx \approx \frac{h}{2}\left[f(a) + 2\sum_{i=1}^{n-1} f(a+ih) + f(b)\right] = h\sum_{i=0}^{n}{}'' f(a+ih). \tag{6.13}$$

The notation of a sum with two primes, $\sum''$, means that we sum over all the terms with the exception of the first and last terms that are being divided by 2.

We can also compute the error term as a function of the distance between neighboring points, h. We know from (6.11) that in every subinterval the quadrature error is

$$-\frac{h^3}{12}f''(\xi_x).$$

Hence, the overall error is obtained by summing over n such terms:

$$\sum_{i=1}^{n} -\frac{h^3}{12}f''(\xi_i) = -\frac{h^3 n}{12}\left[\frac{1}{n}\sum_{i=1}^{n} f''(\xi_i)\right].$$

Here, we use the notation ξ_i to denote an intermediate point that belongs to the i^{th} interval. Let

$$M = \frac{1}{n}\sum_{i=1}^{n} f''(\xi_i).$$

Clearly

$$\min_{x\in[a,b]} f''(x) \leqslant M \leqslant \max_{x\in[a,b]} f''(x)$$

If we assume that $f''(x)$ is continuous in $[a,b]$ (which we anyhow do in order for the interpolation error formula to be valid) then there exists a point $\xi \in [a,b]$ such that

$$f''(\xi) = M.$$

Hence (recalling that $(b-a)/n = h$, we have

$$E = -\frac{(b-a)h^2}{12}f''(\xi), \qquad \xi \in [a,b]. \tag{6.14}$$

This means that the composite trapezoidal rule is second-order accurate.

Example 6.3
In the interval $[a,b]$ we assume n subintervals and let

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

The quadrature points are

$$x_j = a + \left(j - \frac{1}{2}\right)h, \qquad j = 1, 2, \ldots, n.$$

The composite midpoint rule is given by applying the midpoint rule (6.4) in every subinterval, i.e.,

$$\int_a^b f(x)dx \approx h \sum_{j=1}^{n} f(x_j). \tag{6.15}$$

Equation (6.15) is known as **the composite midpoint rule**.

In order to obtain the quadrature error in the approximation (6.15) we recall that in each subinterval the error is given according to (6.6), i.e.,

$$E_j = \frac{h^3}{24} f''(\xi_j), \qquad \xi_j \in \left(x_j - \frac{h}{2}, x_j + \frac{h}{2}\right).$$

Hence

$$E = \sum_{j=1}^{n} E_j = \frac{h^3}{24} \sum_{j=1}^{n} f''(\xi_j) = \frac{h^3}{24} n \left[\frac{1}{n} \sum_{j=1}^{n} f''(\xi_j)\right] = \frac{h^2(b-a)}{24} f''(\xi), \tag{6.16}$$

where $\xi \in (a, b)$. This means that the composite midpoint rule is also second-order accurate (just like the composite trapezoidal rule).

6.4 Additional Integration Techniques

6.4.1 The method of undetermined coefficients

The methods of undetermined coefficients for deriving quadratures is the following:

1. Select the quadrature points.
2. Write a quadrature as a linear combination of the values of the function at the chosen quadrature points.
3. Determine the coefficients of the linear combination by requiring that the quadrature is *exact* for as many polynomials as possible from the the ordered set $\{1, x, x^2, \ldots\}$.

We demonstrate this technique with the following example.

Example 6.4
Problem: Find a quadrature of the form

$$\int_0^1 f(x)dx \approx A_0 f(0) + A_1 f\left(\frac{1}{2}\right) + A_2 f(1),$$

that is exact for all polynomials of degree $\leqslant 2$.

Solution: Since the quadrature has to be exact for all polynomials of degree $\leqslant 2$, it has to be exact for the polynomials 1, x, and x^2. Hence we obtain the system of linear equations

$$\begin{aligned} 1 &= \int_0^1 1dx = A_0 + A_1 + A_2, \\ \frac{1}{2} &= \int_0^1 xdx = \frac{1}{2}A_1 + A_2, \\ \frac{1}{3} &= \int_0^1 x^2dx = \frac{1}{4}A_1 + A_2. \end{aligned}$$

Therefore, $A_0 = A_2 = \frac{1}{6}$ and $A_1 = \frac{2}{3}$, and the desired quadrature is

$$\int_0^1 f(x)dx \approx \frac{f(0) + 4f\left(\frac{1}{2}\right) + f(1)}{6}. \tag{6.17}$$

Since the resulting formula (6.17) is linear, its being exact for 1, x, and x^2, implies that it is exact for any polynomial of degree $\leqslant 2$. In fact, we will show in Section 6.5.1 that this approximation is actually exact for polynomials of degree $\leqslant 3$.

6.4.2 Change of an interval

Suppose that we have a quadrature formula on the interval $[c, d]$ of the form

$$\int_c^d f(t)dt \approx \sum_{i=0}^n A_i f(t_i). \tag{6.18}$$

We would like to to use (6.18) to find a quadrature on the interval $[a, b]$, that approximates for

$$\int_a^b f(x)dx.$$

The mapping between the intervals $[c, d] \to [a, b]$ can be written as a linear transformation of the form

$$\lambda(t) = \frac{b-a}{d-c}t + \frac{ad-bc}{d-c}.$$

Hence

$$\int_a^b f(x)dx = \frac{b-a}{d-c}\int_c^d f(\lambda(t))dt \approx \frac{b-a}{d-c}\sum_{i=0}^n A_i f(\lambda(t_i)).$$

This means that

$$\int_a^b f(x)dx \approx \frac{b-a}{d-c}\sum_{i=0}^n A_i f\left(\frac{b-a}{d-c}t_i + \frac{ad-bc}{d-c}\right). \tag{6.19}$$

We note that if the quadrature (6.18) was exact for polynomials of degree m, so is (6.19).

Example 6.5
We want to write the result of the previous example

$$\int_0^1 f(x)dx \approx \frac{f(0) + 4f\left(\frac{1}{2}\right) + f(1)}{6},$$

as a quadrature on the interval $[a, b]$. According to (6.19)

$$\int_a^b f(x)dx \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]. \tag{6.20}$$

The approximation (6.20) is known as the **Simpson quadrature**.

6.5 Simpson's Integration

In the last example we obtained Simpson's quadrature (6.20). An alternative derivation is the following: start with a polynomial $Q_2(x)$ that interpolates $f(x)$ at the points a, $(a+b)/2$, and b. Then approximate

$$\begin{aligned}\int_a^b f(x)dx \quad &\approx \quad \int_a^b \left[\frac{(x-c)(x-b)}{(a-c)(a-b)}f(a) + \frac{(x-a)(x-b)}{(c-a)(c-b)}f(c) + \frac{(x-a)(x-c)}{(b-a)(b-c)}f(b)\right]dx \\ &= \ldots = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right],\end{aligned}$$

which is Simpson's rule (6.20). Figure 6.5 demonstrates this process of deriving Simpson's quadrature for the specific choice of approximating $\int_1^3 \sin x dx$.

6.5.1 The quadrature error

It turns out that Simpson's quadrature is exact for polynomials of degree $\leqslant 3$ and not only for polynomials of degree $\leqslant 2$, as expected by the way it was constructed. We will obtain this result by studying the error term.

In order to derive the error term for Simpson's method, we discuss an error analysis technique that is valid for quadratures that are obtained through integration. In all such cases, the quadrature error is the difference between the integral of the function and the integral of its interpolant, i.e.,

$$E = \int_a^b (f(t) - p_n(t))dt = \int_a^b \frac{f^{(n+1)}(\xi_x)}{(n+1)!}\omega(t)dt, \tag{6.21}$$

where

$$\omega(t) = \prod_{i=0}^{n}(t - t_i)dt.$$

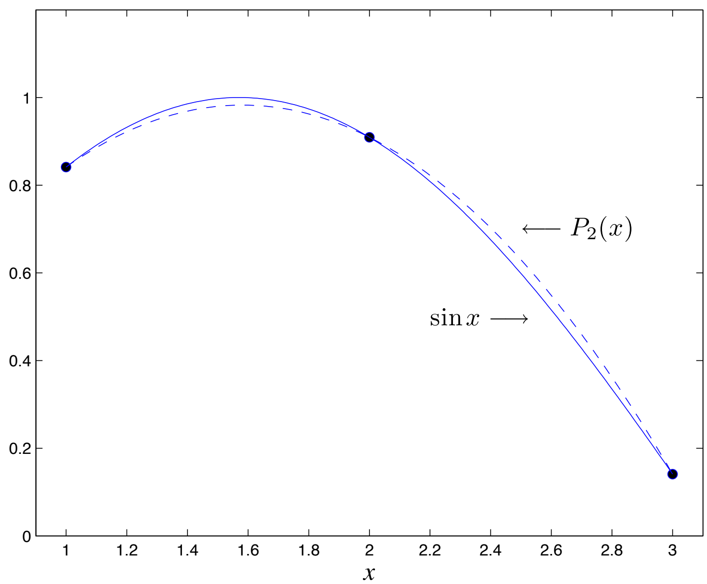

Figure 6.5: An example of Simpson's quadrature. The approximation of $\int_1^3 \sin x dx$ is obtained by integrating the quadratic interpolant $Q_2(x)$ over $[1, 3]$

It $\omega(t)$ is always non-negative or non-positive between a and b, then according to the midvalue theorem for integrals, the error in (6.21) becomes

$$E = \frac{f^{(n+1)}(\xi)}{(n+1)!} \int_a^b \omega(t) dt, \qquad \xi \in (a, b).$$

Examples for such cases are the trapezoidal rule for which

$$E = \frac{f''(\xi)}{12}(b-a)^3,$$

and the rectangle rule for which

$$E = \frac{f'(\xi)}{1} \int_a^b (t-a) dt = \frac{f'(\xi)}{2}(b-a)^2.$$

Another case which is rather easy to analyze is the case in which

$$\int_a^b \omega(t) dt = 0. \tag{6.22}$$

Examples for the case in (6.22) include the midpoint rule for which

$$\int_a^b \omega(t) dt = \int_a^b \left(t - \frac{a+b}{2}\right) dt = 0,$$

and Simpson's rule for which

$$\int_a^b \omega(t)dt = \int_a^b (t-a)\left(t-\frac{a+b}{2}\right)(t-b)dt = 0.$$

In this case, we can add another interpolation point without changing the integral of the interpolant. This is the case since we replace $f(x)$ by $p_n(x)$ and integrate

$$\int_a^b f(t)dt \approx \int_a^b p_n(x)dx.$$

Adding an arbitrary interpolation point, x_{n+1}, to $p_n(x)$ turns it into an interpolating polynomial of a higher order, $p_{n+1}(x)$, that is given by

$$p_{n+1}(x) = p_n(x) + f[x_0, \ldots, x_{n+1}]\omega(x). \tag{6.23}$$

Since $\int_a^b \omega(x)dx = 0$, when integrating (6.23) in order to obtain a quadrature, we observe that

$$\int_a^b f(t)dt \approx \int_a^b p_{n+1}(x)dx = \int_a^b p_n(x)dx,$$

so the original quadrature does not change by adding an arbitrary interpolation point.

We now have all the required tools in order to derive a quadrature for Simpson's method. Since in this case $\int_a^b \omega(t)dt = 0$, we add to $a, \frac{a+b}{2}, b$ an arbitrary interpolation point which we choose as $\frac{a+b}{2}$ again. The function $\omega(t)$ becomes

$$\omega(t) = (t-a)\left(t-\frac{a+b}{2}\right)^2(t-b).$$

Hence, for $t \in [a,b]$, our new $\omega(t)$ satisfies $\omega(t) \leqslant 0$. By the midvalue theorem for integrals the error in Simpson's method can be written as

$$E = \frac{f^{(4)}(\xi)}{24}\int_a^b (t-a)\left(t-\frac{a+b}{2}\right)^2(t-b)dt = -\frac{1}{90}\left(\frac{b-a}{2}\right)^5 f^{(4)}(\xi), \tag{6.24}$$

for $\xi \in (a,b)$. Since the fourth derivative of any polynomial of degree $\leqslant 3$ is identically zero, the quadrature error formula (6.24) implies that Simpson's quadrature is exact for polynomials of degree $\leqslant 3$.

6.5.2 Composite Simpson rule

To derive a composite version of Simpson's quadrature, we divide the interval $[a,b]$ into an even number of subintervals, n, and let

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

where

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

Hence, if we replace the integral in every subintervals by Simpson's rule (6.20), we obtain

$$\begin{aligned}\int_a^b f(x)dx &= \int_{x_0}^{x_2} f(x)dx + \ldots + \int_{x_{n-2}}^{x_n} f(x)dx = \sum_{i=1}^{n/2} \int_{x_{2i-2}}^{x_{2i}} f(x)dx \\ &\approx \frac{h}{3}\sum_{i=1}^{n/2}\left[f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})\right].\end{aligned}$$

The **composite Simpson quadrature** is thus given by

$$\int_a^b f(x)dx \approx \frac{h}{3}\left[f(x_0) + 2\sum_{i=0}^{n/2} f(x_{2i-2}) + 4\sum_{i=1}^{n/2} f(x_{2i-1}) + f(x_n)\right]. \tag{6.25}$$

Summing the error terms (that are given by (6.24)) over all sub-intervals, the quadrature error takes the form

$$E = -\frac{h^5}{90}\sum_{i=1}^{n/2} f^{(4)}(\xi_i) = -\frac{h^5}{90}\cdot\frac{n}{2}\cdot\frac{2}{n}\sum_{i=1}^{n/2} f^{(4)}(\xi_i).$$

Since

$$\min_{x\in[a,b]} f^{(4)}(x) \leqslant \frac{2}{n}\sum_{i=1}^{n/2} f^{(4)}(\xi_i) \leqslant \max_{x\in[a,b]} f^{(4)}(x),$$

we can conclude that

$$E = -\frac{h^5}{90}\frac{n}{2}f^{(4)}(\xi) = -\frac{h^4}{180}f^{(4)}(\xi), \qquad \xi \in [a,b], \tag{6.26}$$

i.e., the composite Simpson quadrature is fourth-order accurate.

6.6 Weighted Quadratures

We recall that a weight function is a continuous, non-negative function with a positive mass. We assume that such a weight function $w(x)$ is given and would like to write a quadrature of the form

$$\int_a^b f(x)w(x)dx \approx \sum_{i=0}^{n} A_i f(x_i). \tag{6.27}$$

Such quadratures are called **general (weighted) quadratures**.

Previously, for the case $w(x) \equiv 1$, we wrote a quadrature of the form

$$\int_a^b f(x)dx \approx \sum_{i=0}^n A_i f(x_i),$$

where

$$A_i = \int_a^b l_i(x)dx.$$

Repeating the derivation we carried out in Section 6.2, we construct an interpolant $Q_n(x)$ of degree $\leqslant n$ that passes through the points $x_0, \ldots, x_n$. Its Lagrange form is

$$Q_n(x) = \sum_{i=0}^n f(x_i) l_i(x),$$

with the usual

$$l_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^n \frac{x - x_j}{x_i - x_j}, \qquad 0 \leqslant i \leqslant n.$$

Hence

$$\int_a^b f(x)w(x)dx \approx \int_a^b Q_n(x)w(x)dx = \sum_{i=0}^n f(x_i) \int_a^b l_i(x)w(x)dx = \sum_{i=0}^n A_i f(x_i),$$

where the coefficients A_i are given by

$$A_i = \int_a^b l_i(x)w(x)dx. \tag{6.28}$$

To summarize, the general quadrature is

$$\int_a^b f(x)w(x)dx \approx \sum_{i=0}^n A_i f(x_i), \tag{6.29}$$

with quadrature coefficients, A_i, that are given by (6.28).

6.7 Gaussian Quadrature

6.7.1 Maximizing the quadrature's accuracy

So far, all the quadratures we encountered were of the form

$$\int_a^b f(x)dx \approx \sum_{i=0}^n A_i f(x_i). \tag{6.30}$$

An approximation of the form (6.30) was shown to be exact for polynomials of degree $\leqslant n$ for an appropriate choice of the quadrature coefficients A_i. In all cases, the quadrature points $x_0, \ldots, x_n$ were given up front. In other words, given a set of nodes $x_0, \ldots, x_n$, the coefficients $\{A_i\}_{i=0}^n$ were determined such that the approximation was exact in Π_n.

We are now interested in investigating the possibility of writing more accurate quadratures without increasing the total number of quadrature points. This will be possible if we allow for the freedom of choosing the quadrature points. The quadrature problem becomes now a problem of choosing the quadrature points in addition to determining the corresponding coefficients in a way that the quadrature is exact for polynomials of a maximal degree. Quadratures that are obtained that way are called **Gaussian quadratures**.

Example 6.6
The quadrature formula

$$\int_{-1}^{1} f(x)dx \approx f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right),$$

is exact for polynomials of degree $\leqslant 3$(!) We will revisit this problem and prove this result in Example 6.9 below.

An equivalent problem can be stated for the more general weighted quadrature case. Here,

$$\int_a^b f(x)w(x)dx \approx \sum_{i=0}^n A_i f(x_i), \tag{6.31}$$

where $w(x) \geqslant 0$ is a weight function. Equation (6.31) is exact for $f \in \Pi_n$ if and only if

$$A_i = \int_a^b w(x) \prod_{\substack{j=0 \\ j\neq i}} \frac{x - x_j}{x_i - x_j} dx. \tag{6.32}$$

In both cases (6.30) and (6.31), the number of quadrature nodes, $x_0, \ldots, x_n$, is $n+1$, and so is the number of quadrature coefficients, A_i. Hence, if we have the flexibility of determining the location of the points in addition to determining the coefficients, we have altogether $2n+2$ degrees of freedom, and hence we can expect to be able to derive quadratures that are exact for polynomials in Π_{2n+1}. This is indeed the case as we shall see below. We will show that the general solution of this integration problem is connected with the roots of orthogonal polynomials. We start with the following theorem.

Theorem 6.7 *Let $q(x)$ be a nonzero polynomial of degree $n+1$ that is w-orthogonal to Π_n, i.e., $\forall p(x) \in \Pi_n$,*

$$\int_a^b p(x)q(x)w(x)dx = 0.$$

If $x_0, \ldots, x_n$ are the zeros of $q(x)$ then (6.31), with A_i given by (6.32), is exact $\forall f \in \Pi_{2n+1}$.

Proof. For $f(x) \in \Pi_{2n+1}$, write $f(x) = q(x)p(x) + r(x)$. We note that $p(x), r(x) \in \Pi_n$. Since $x_0, \ldots, x_n$ are the zeros of $q(x)$ then

$$f(x_i) = r(x_i).$$

Hence,

$$\begin{aligned}\int_a^b f(x)w(x)dx &= \int_a^b [q(x)p(x) + r(x)]w(x)dx = \int_a^b r(x)w(x)dx \\ &= \sum_{i=0}^n A_i r(x_i) = \sum_{i=0}^n A_i f(x_i).\end{aligned} \tag{6.33}$$

The second equality in (6.33) holds since $q(x)$ is w-orthogonal to Π_n. The third equality (6.33) holds since (6.31), with A_i given by (6.32), is exact for polynomials in Π_n. ■

According to Theorem 6.7 we already know that the quadrature points that will provide the most accurate quadrature rule are the $n+1$ roots of an orthogonal polynomial of degree $n+1$ (where the orthogonality is with respect to the weight function $w(x)$). We recall that the roots of $q(x)$ are real, simple and lie in (a, b), something we know from our previous discussion on orthogonal polynomials (see Theorem **??**). In other words, we need $n+1$ quadrature points in the interval, and an orthogonal polynomial of degree $n+1$ does have $n+1$ distinct roots in the interval. We now restate the result regarding the roots of orthogonal functions with an alternative proof.

Theorem 6.8 *Let $w(x)$ be a weight function. Assume that $f(x)$ is continuous in $[a, b]$ that is not the zero function, and that $f(x)$ is w-orthogonal to Π_n. Then $f(x)$ changes sign at least $n+1$ times on (a, b).*

Proof. Since $1 \in \Pi_n$,

$$\int_a^b f(x)w(x)dx = 0.$$

Hence, $f(x)$ changes sign at least once. Now suppose that $f(x)$ changes size only r times, where $r \leqslant n$. Choose $\{t_i\}_{i \geqslant 0}$ such that

$$a = t_0 < t_1 < \cdots < t_r = b,$$

and $f(x)$ is of one sign on $(t_0, t_1), (t_1, t_2), \ldots, (t_{r-1}, t_r)$. The polynomial

$$p(x) = \prod_{i=0}^{r-1} (x - t_i),$$

has the same sign property. Hence

$$\int_a^b f(x)p(x)w(x)dx \neq 0,$$

which leads to a contradiction since $p(x) \in \Pi_n$. ■

Example 6.9
We are looking for a quadrature of the form

$$\int_{-1}^{1} f(x)dx \approx A_0 f(x_0) + A_1 f(x_1).$$

A straightforward computation will amount to making this quadrature exact for the polynomials of degree $\leqslant 3$. The linearity of the quadrature means that it is sufficient to make the quadrature exact for 1, x, x^2, and x^3. Hence we write the system of equations

$$\int_{-1}^{1} f(x)dx = \int_{-1}^{1} x^i dx = A_0 x_0^i + A_1 x_1^i, \qquad i = 0, 1, 2, 3.$$

From this we can write

$$\begin{cases} A_0 + A_1 = 2, \\ A_0 x_0 + A_1 x_1 = 0, \\ A_0 x_0^2 + A_1 x_1^2 = \frac{2}{3}, \\ A_0 x_0^3 + A_1 x_1^3 = 0. \end{cases}$$

Solving for A_1, A_2, x_0, and x_1 we get

$$A_1 = A_2 = 1, \qquad x_0 = -x_1 = \frac{1}{\sqrt{3}},$$

so that the desired quadrature is

$$\int_{-1}^{1} f(x)dx \approx f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right). \tag{6.34}$$

Example 6.10
We repeat the previous problem using orthogonal polynomials. Since $n = 1$, we expect to find a quadrature that is exact for polynomials of degree $2n+1 = 3$. The polynomial of degree $n+1 = 2$ which is orthogonal to $\Pi_n = \Pi_1$ with weight $w(x) \equiv 1$ is the Legendre polynomial of degree 2, i.e.,

$$P_2(x) = \frac{1}{2}(3x^2 - 1).$$

The integration points will then be the zeros of $P_2(x)$, i.e.,

$$x_0 = -\frac{1}{\sqrt{3}}, \qquad x_1 = \frac{1}{\sqrt{3}}.$$

All that remains is to determine the coefficients A_1, A_2. This is done in the usual way, assuming that the quadrature

$$\int_{-1}^{1} f(x)dx \approx A_0 f(x_0) + A_1 f(x_1),$$

is exact for polynomials of degree $\leqslant 1$. The simplest will be to use 1 and x, i.e.,

$$2 = \int_{-1}^{1} 1dx = A_0 + A_1,$$

and

$$0 = \int_{-1}^{1} xdx = -A_0\frac{1}{\sqrt{3}} + A_1\frac{1}{\sqrt{3}}.$$

Hence $A_0 = A_1 = 1$, and the quadrature is the same as (6.34) (as should be).

6.7.2 Convergence and error analysis

Lemma 6.11 *In a Gaussian quadrature formula, the coefficients are positive and their sum is* $\int_a^b w(x)dx$.

Proof. Fix n. Let $q(x) \in \Pi_{n+1}$ be w-orthogonal to Π_n. Also assume that $q(x_i) = 0$ for $i = 0, \ldots, n$, and take $\{x_i\}_{i=0}^n$ to be the quadrature points, i.e.,

$$\int_a^b f(x)w(x)dx \approx \sum_{i=0}^{n} A_i f(x_i). \tag{6.35}$$

Fix $0 \leqslant j \leqslant n$. Let $p(x) \in \Pi_n$ be defined as

$$p(x) = \frac{q(x)}{x - x_j}.$$

Since x_j is a root of $q(x)$, $p(x)$ is indeed a polynomial of degree $\leqslant n$. The degree of $p^2(x) \leqslant 2n$ which means that the Gaussian quadrature (6.35) is exact for it. Hence

$$0 < \int_a^b p^2(x)w(x)dx = \sum_{i=0}^{n} A_i p^2(x_i) = \sum_{i=0}^{n} A_i \frac{q^2(x_i)}{(x_i - x_j)^2} = A_j p^2(x_j),$$

which means that $\forall j$, $A_j > 0$. In addition, since the Gaussian quadrature is exact for $f(x) \equiv 1$, we have

$$\int_a^b w(x)dx = \sum_{i=0}^n A_i. \qquad \blacksquare$$

In order to estimate the error in the Gaussian quadrature we would first like to present an alternative way of deriving the Gaussian quadrature. Our starting point is the Lagrange form of the Hermite polynomial that interpolates $f(x)$ and $f'(x)$ at $x_0, \ldots, x_n$. It is given by (??), i.e.,

$$p(x) = \sum_{i=0}^n f(x_i)a_i(x) + \sum_{i=0}^n f'(x_i)b_i(x),$$

with

$$a_i(x) = (l_i(x))^2[1 + 2l_i'(x_i)(x_i - x)], \qquad b_i(x) = (x - x_i)l_i^2(x), \qquad 0 \leq i \leq n,$$

and

$$l_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^n \frac{x - x_j}{x_i - x_j}.$$

We now assume that $w(x)$ is a weight function in $[a, b]$ and approximate

$$\int_a^b w(x)f(x)dx \approx \int_a^b w(x)p_{2n+1}(x)dx = \sum_{i=0}^n A_i f(x_i) + \sum_{i=0}^n B_i f'(x_i), \tag{6.36}$$

where

$$A_i = \int_a^b w(x)a_i(x)dx, \tag{6.37}$$

and

$$B_i = \int_a^b w(x)b_i(x)dx. \tag{6.38}$$

In some sense, it seems to be rather strange to deal with the Hermite interpolant when we do not explicitly know the values of $f'(x)$ at the interpolation points. However, we can eliminate the derivatives from the quadrature (6.36) by setting $B_i = 0$ in (6.38). Indeed (assuming $n \neq 0$):

$$B_i = \int_a^b w(x)(x - x_i)l_i^2(x)dx = \prod_{\substack{j=0 \\ j \neq i}}^n (x_i - x_j) \int_a^b w(x) \prod_{j=0}^n (x - x_j) l_i(x)dx.$$

Hence, $B_i = 0$, if the product $\prod_{j=0}^{n}(x - x_j)$ is orthogonal to $l_i(x)$. Since $l_i(x)$ is a polynomial in Π_n, all that we need is to set the points $x_0, \ldots, x_n$ as the roots of a polynomial of degree $n+1$ that is w-orthogonal to Π_n. This is precisely what we defined as a Gaussian quadrature.

We are now ready to formally establish the fact that the Gaussian quadrature is exact for polynomials of degree $\leqslant 2n+1$.

Theorem 6.12 *Let $f \in C^{2n+2}[a,b]$ and let $w(x)$ be a weight function. Consider the Gaussian quadrature*

$$\int_a^b f(x)w(x)dx \approx \sum_{i=0}^{n} A_i f(x_i).$$

Then there exists $\zeta \in (a,b)$ such that

$$\int_a^b f(x)w(x)dx - \sum_{i=0}^{n} A_i f(x_i) = \frac{f^{(2n+2)}(\zeta)}{(2n+2)!}\int_a^b \prod_{j=0}^{n}(x - x_j)^2 w(x)dx.$$

Proof. We use the characterization of the Gaussian quadrature as the integral of a Hermite interpolant. We recall that the error formula for the Hermite interpolation is given by (**??**),

$$f(x) - p_{2n+1}(x) = \frac{f^{(2n+2)}(\xi)}{(2n+2)!}\prod_{j=0}^{n}(x - x_j)^2, \qquad \xi \in (a,b).$$

Hence according to (6.36) we have

$$\begin{aligned}\int_a^b f(x)w(x)dx - \sum_{i=0}^{n} A_i f(x_i) &= \int_a^b f(x)w(x)dx - \int_a^b p_{2n+1}w(x)dx \\ &= \int_a^b w(x)\frac{f^{(2n+2)}(\xi)}{(2n+2)!}\prod_{j=0}^{n}(x - x_j)^2 dx.\end{aligned}$$

The integral mean value theorem then implies that there exists $\zeta \in (a,b)$ such that

$$\int_a^b f(x)w(x)dx - \sum_{i=0}^{n} A_i f(x_i) = \frac{f^{(2n+2)}(\zeta)}{(2n+2)!}\int_a^b \prod_{j=0}^{n}(x - x_j)^2(x)w(x)dx. \quad \blacksquare$$

We conclude this section with a convergence theorem that states that for continuous functions, the Gaussian quadrature converges to the exact value of the integral as the number of quadrature points tends to infinity. This theorem is not of a great practical value because it does not provide an estimate on the rate of convergence. A proof of the theorem that is based on the Weierstrass approximation theorem can be found in, e.g., in [**?**].

Theorem 6.13 *We let $w(x)$ be a weight function and assuming that $f(x)$ is a continuous function on $[a,b]$. For each $n \in \mathbb{N}$ we let $\{x_{n_i}\}_{i=0}^n$ be the $n+1$ roots of the polynomial of degree $n+1$ that is w-orthogonal to Π_n, and consider the corresponding Gaussian quadrature:*

$$\int_a^b f(x)w(x)dx \approx \sum_{i=0}^n A_{n_i} f(x_{n_i}). \tag{6.39}$$

Then the right-hand-side of (6.39) converges to the left-hand-side as $n \to \infty$.

6.8 Romberg Integration

We have introduced Richardson's extrapolation in Section **??** in the context of numerical differentiation. We can use a similar principle with numerical integration.

We will demonstrate this principle with a particular example. Let I denote the exact integral that we would like to approximate, i.e.,

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

Let's assume that this integral is approximated with a composite trapezoidal rule on a uniform grid with mesh spacing h (6.13),

$$T(h) = h \sum_{i=0}^{n}{}'' f(a+ih).$$

We know that the composite trapezoidal rule is second-order accurate (see (6.14)). A more detailed study of the quadrature error reveals that the difference between I and $T(h)$ can be written as

$$I = T(h) + c_1 h^2 + c_2 h^4 + \ldots + c_k h^k + O(h^{2k+2}).$$

The exact values of the coefficients, c_k, are of no interest to us as long as they do not depend on h (which is indeed the case). We can now write a similar quadrature that is based on half the number of points, i.e., $T(2h)$. Hence

$$I = T(2h) + c_1(2h)^2 + c_2(2h)^4 + \ldots$$

This enables us to eliminate the h^2 error term:

$$I = \frac{4T(h) - T(2h)}{3} + \hat{c}_2 h^4 + \ldots$$

Therefore

$$\begin{aligned}\frac{4T(h)-T(2h)}{3} &= \frac{1}{3}\left[4h\left(\frac{1}{2}f_0+f_1+\ldots+f_{n-1}+\frac{1}{2}f_n\right)\right.\\ &\left.-2h\left(\frac{1}{2}f_0+f_2+\ldots+f_{n-2}+\frac{1}{2}f_n\right)\right]\\ &= \frac{h}{3}\left(f_0+4f_1+2f_2+\ldots+2f_{n-2}+4f_{n-1}+f_n\right)=S(n).\end{aligned}$$

Here, $S(n)$ denotes the composite Simpson's rule with n subintervals. The procedure of increasing the accuracy of the quadrature by eliminating the leading error term is known as **Romberg integration**. In some places, Romberg integration is used to describe the specific case of turning the composite trapezoidal rule into Simpson's rule (and so on). The quadrature that is obtained from Simpson's rule by eliminating the leading error term is known as the **super Simpson rule**.