Chapter 4. Numerical Differentiation and Integration

1 Approximation of Linear Functionals, Basic Notions

Let X be a linear space and $L, L_1, \ldots, L_m : X \to \mathbb{R}$ be real, linear functionals, that are linearly independent.

Definition 1.1. *An approximation formula of L using $L_1, \ldots, L_m$, is a formula of the type*

$$L(f) = \sum_{i=1}^{m} A_i L_i(f) + R(f), \; f \in X. \tag{1.1}$$

*The real parameters A_i are called **coefficients**, and $R(f)$ is the **remainder** of the formula.*

For an approximation formula of the form (1.1), given L_i, we want to determine the coefficients A_i and study the corresponding remainder (error).
The functionals L_i express the available information on f and they also depend on the particular type of approximation we seek, i.e. on L.

Example 1.2. Let $X = \{f \mid f : [a, b] \to \mathbb{R}\}$, $L_i(f) = f(x_i)$, for some distinct nodes $x_i \in [a, b], i = \overline{0, m}$ and $L(f) = f(\alpha)$, for an arbitrary $\alpha \in [a, b]$. Formula (1.1) becomes

$$f(\alpha) = \sum_{i=0}^{m} l_i(\alpha) f(x_i) + (Rf)(\alpha),$$

i.e. the *Lagrange interpolation formula*. We have

$$A_i = l_i(\alpha),$$

where l_i are the Lagrange fundamental polynomials. One of the expressions for the remainder is

$$(Rf)(\alpha) = \frac{u(\alpha)}{(m+1)!} f^{(m+1)}(\xi), \; \xi \in [a, b], \; u(x) = (x - x_0) \ldots (x - x_m),$$

if $f^{(m+1)}$ exists on $[a, b]$.

Example 1.3. Let X and L_i be defined as in the previous example. Assuming that $f^{(k)}(\alpha), \; k \in \mathbb{N}^*$ exists, define $L(f) = f^{(k)}(\alpha)$. We get an approximation formula for the derivative of order k of f

at α,

$$f^{(k)}(\alpha) = \sum_{i=0}^{m} A_i f(x_i) + R(f),$$

called a *numerical differentiation formula*.

Example 1.4. Let $x_k \in [a,b], k = \overline{0,m}$ be distinct nodes and I_k some sets of indices. Consider $X = \{f \mid f : [a,b] \to \mathbb{R}, f$ integrable on $[a,b]$, for which $f^{(j)}(x_k), k = \overline{0,m}, j \in I_k$ exist$\}$, $L_{kj}(f) = f^{(j)}(x_k)$ and $L(f) = \int\limits_a^b f(x)dx$. Formula (1.1) becomes

$$\int\limits_a^b f(x)dx = \sum_{k=0}^{m} \sum_{j \in I_k} A_{kj} f^{(j)}(x_k) + R(f),$$

called a *numerical integration (quadrature) formula*.

In general, there are two approaches for solving the approximation problem (1.1):
$-$ the **interpolation method**: apply the functional L to a suitable interpolation polynomial of f, instead of f itself;
$-$ the **method of undetermined coefficients**: find the coefficients in (1.1), by making the remainder $R(f)$ be 0 for polynomials of degree as high as possible, i.e., imposing the conditions $R(e_k) = 0,\ e_k(x) = x^k,\ k = 0, 1, \ldots, d$, for as large a d as possible.

2 Numerical Differentiation

Numerical approximation of derivatives is used when the values of a function f are given in tables, as empirical data, or the expression of f is complicated.
We can derive simple, immediate numerical differentiation rules using divided and finite differences.
Let $f : [a,b] \to \mathbb{R}$ be differentiable on $[a,b], x \in [a,b]$, arbitrary and $h > 0$. We have

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} = \lim_{h \to 0} f[x, x+h].$$

From here, we immediately get the approximation

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \equiv D_h f(x), \tag{2.1}$$

called the *forward difference numerical derivative*.

Expanding $f(x+h)$ in a Taylor's series around x, we get

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2} f''(\xi), \\ \frac{f(x+h)-f(x)}{h} &= f'(x) + \frac{h}{2} f''(\xi),\ \xi \in (x, x+h), \end{aligned}$$

from which we have the error formula

$$(RD_h f)(x) \;=\; f'(x) - D_h f(x) \;=\; -\frac{h}{2} f''(\xi),\ \xi \in (x, x+h). \tag{2.2}$$

The error is proportional to h, so formula (2.2) can be used for small steps h.

Similarly, we obtain the *backward difference numerical derivative*,

$$f'(x) \;\approx\; \frac{f(x)-f(x-h)}{h} \;\equiv\; \widetilde{D}_h f(x), \tag{2.3}$$

with approximation error

$$(R\widetilde{D}_h f)(x) \;=\; f'(x) - \frac{f(x)-f(x-h)}{h} \;=\; \frac{h}{2} f''(\xi),\ \xi \in (x-h, x). \tag{2.4}$$

Interpolating f at the nodes $x-h,\ x+h$ and then taking the derivative, we obtain

$$f'(x) \;\approx\; \frac{f(x+h)-f(x-h)}{2h} \;\equiv\; \widehat{D}_h f(x), \tag{2.5}$$

known as the *central difference numerical derivative formula*, with remainder given by

$$(R\widehat{D}_h f)(x) \;=\; -\frac{h^2}{6} f'''(\xi),\ \xi \in (x-h, x+h). \tag{2.6}$$

This says that for small values of h, the formula (2.5) should be more accurate than the earlier approximations, because the error term of (2.6) decreases more rapidly with h.

Example 2.1. Use $D_h f$ and $\widehat{D}_h f$ to approximate the derivative of $f(x) = \cos x$ at $x = \pi/6$. Study the error of each approximation.

Solution. The exact value is $f'\left(\frac{\pi}{6}\right) \;=\; -\sin\frac{\pi}{6} \;=\; -\frac{1}{2}$.

By (2.2), when using $D_h f$,the error is

$$(RD_h f)\left(\frac{\pi}{6}\right) \;=\; f'\left(\frac{\pi}{6}\right) - D_h\left(\frac{\pi}{6}\right) \;=\; \frac{h}{2}\cos\xi,$$

thus,

$$\left|(RD_h f)\left(\frac{\pi}{6}\right)\right| \;\leq\; \frac{h}{2}.$$

Similarly, for $\widehat{D}_h f$, the error is bounded by

$$\left|(R\widehat{D}_h f)\left(\frac{\pi}{6}\right)\right| \;\leq\; \frac{h^2}{6}.$$

Table 1 contains the approximation results yielded by the two methods, for various values of h. Indeed, both the value of $D_h f$ and that of $\widehat{D}_h f$ are approaching -0.5. Moreover, looking at the errors, we see that when h is halved, the error is almost halved (see the first ratio column) for the first approximation. This confirms the fact that the error is proportional to h (relation (2.2)). For the approximation $\widehat{D}_h f$, we see that the errors decrease more rapidly and the last column of ratios confirms the (superior) rate of convergence of $O(h^2)$ given in (2.6).

h	$D_h f$	Error	Ratio	$\widehat{D}_h f$	Error	Ratio
0.1	-0.54243	$4.243e-2$		-0.49917	$-8.329e-4$	
0.05	-0.52144	$2.144e-2$	1.98	-0.49979	$-2.083e-4$	4.00
0.025	-0.51077	$1.077e-2$	1.99	-0.49995	$-5.208e-5$	4.00
0.0125	-0.50540	$5.403e-3$	1.99	-0.49998	$-1.302e-5$	4.00
0.00625	-0.50270	$2.701e-3$	2.00	-0.49999	$-3.255e-6$	4.00

Table 1: Example 2.1, $f(x) = \cos x$

■

Remark 2.2. One must be very cautious in using numerical differentiation, because of the sensitivity to errors in the function values. This is especially true if the function values are obtained empirically with relatively large experimental errors, as is common in practice. Numerical differentiation is an *unstable* operation, meaning that even if the approximation of a function is good, that *does not* guarantee that its derivative will be a good approximation for the derivative of the function.

Here is such an example: Let

$$f(x) \;=\; g(x) + \frac{x^{n^2}}{n},\ n \geq 1,\ x \in [0,1],\ f, g \in C[0,1].$$

Notice that

$$\begin{aligned} ||f - g||_\infty &= \max_{x \in [0,1]} \frac{x^{n^2}}{n} \;=\; \frac{1}{n} \to 0,\ n \to \infty, \\ ||f' - g'||_\infty &= \max_{x \in [0,1]} n x^{n^2 - 1} \;=\; n \to \infty. \end{aligned}$$

Numerical derivatives can be used to find numerical methods for (ordinary or partial) differential equations. This is done in order to reduce the differential equation to a form that can be solved more easily than the original equation.

3 Numerical Integration

Let $f : [a, b] \to \mathbb{R}$ be integrable on $[a, b]$, $F_k(f), k = \overline{0, m}$ give information on f (usually, linear functionals, such as values or derivatives) and let $w : [a, b] \to \mathbb{R}_+$ be a weight function which is integrable on $[a, b]$.

Definition 3.1. *A formula of the type*

$$\int_a^b w(x) f(x) dx \;=\; \sum_{j=0}^{m} A_j F_j(f) + R(f), \tag{3.1}$$

*is called a **numerical integration formula** for the function f or a **quadrature formula**. The parameters $A_j, j = \overline{0, m}$ are called the **coefficients** of the formula, and $R(f)$ the **remainder**.*

The weight function can be very useful in, among other things, "absorbing" any singularities the integrand has on $[a, b]$ (since on the right-hand-side *only* values related to f are used).

Definition 3.2. *The natural number d satisfying the property that $\forall f \in \mathbb{P}_d, R(f) = 0$ and $\exists g \in \mathbb{P}_{d+1}$ such that $R(g) \neq 0$ is called **degree of precision** (or **degree of exactness**) of the quadrature formula* (3.1).

Remark 3.3. Since R is o linear functional, it follows that a quadrature formula has degree of precision d if and only if

$$R(e_j) \;=\; 0,\; j = 0, 1, \ldots, d,\; R(e_{d+1}) \neq 0. \tag{3.2}$$

If the degree of precision of a quadrature formula is known, then the remainder can be determined using Peano's Theorem.

3.1 Interpolatory Quadratures, Newton-Cotes Formulas

For now, we will restrict our discussion to the case $w(x) \equiv 1$. Many numerical integration formulas are based on the idea of replacing f by an approximating function whose integral can be evaluated. Most of the times, that approximating function is an interpolation polynomial. Then, we obtain a quadrature formula of the form

$$\int_a^b f(x)dx \;=\; \sum_{k=0}^{m} A_k f(x_k) + R(f), \tag{3.3}$$

called an **interpolatory quadrature**. If, in addition, the nodes used are equally spaced, it is called a **Newton-Cotes quadrature**. If the nodes include the endpoints of the interval, a and b, then we have a *closed* Newton-Cotes formula, otherwise, an *open* one.

There are $2m+2$ unknowns ($m+1$ nodes and $m+1$ coefficients) in formula (3.3). Imposing conditions (3.2), it follows that the maximum possible degree of precision can be obtained for a polynomial with $2m+2$ coefficients, i.e. of degree $2m+1$, hence, e_{2m+1}. Thus, the maximum degree of precision of a quadrature formula (3.3) with $m+1$ nodes is

$$d_{\max} \;=\; 2m+1 \;=\; 2 * (\text{nr. of nodes}) - 1.$$

Any interpolatory numerical integration scheme (3.3) has degree of precision at least m (since the interpolation formula has that degree of exactness).

We start with three of the most widely used (but also, simplest) quadratures, obtained from low degree polynomial interpolation.

Rectangle (Midpoint) Rule

We interpolate f at a single *double* node, $x_0 = \dfrac{a+b}{2}$, the midpoint of the interval (hence, the name of the method). So we use the Taylor polynomial of degree 1. Assuming that f has second order continuous derivatives on (a, b), we have

$$\begin{aligned} f(x) &= T_1 f(x) + R_1 f(x) \\ &= f\Big(\frac{a+b}{2}\Big) + \Big(x - \frac{a+b}{2}\Big) f'\Big(\frac{a+b}{2}\Big) + \frac{1}{2!}\Big(x - \frac{a+b}{2}\Big)^2 f''(\xi),\ \xi \in (a, b). \end{aligned}$$

Integrating, we get

$$\begin{aligned} \int_a^b f(x)dx &= (b-a) f\Big(\frac{a+b}{2}\Big) + f'\Big(\frac{a+b}{2}\Big) \int_a^b \Big(x - \frac{a+b}{2}\Big) dx + R(f) \\ &= (b-a) f\Big(\frac{a+b}{2}\Big) + f'\Big(\frac{a+b}{2}\Big) \frac{1}{2}\Big(x - \frac{a+b}{2}\Big)^2 \Big|_a^b + R(f) \\ &= (b-a) f\Big(\frac{a+b}{2}\Big) + R(f), \end{aligned}$$

because the second integral is $\dfrac{1}{2}\Big[\Big(\dfrac{b-a}{2}\Big)^2 - \Big(\dfrac{b-a}{2}\Big)^2\Big] = 0$.
Check the conditions (3.2). We have

$$\begin{aligned} R(e_0) &= \int_a^b e_0(x)dx - (b-a) e_0\Big(\frac{a+b}{2}\Big) \ = \ b - a - (b-a) \ = \ 0, \\ R(e_1) &= \int_a^b x dx - (b-a)\frac{a+b}{2} \ = \ \frac{b^2 - a^2}{2} - \frac{b^2 - a^2}{2} \ = \ 0. \end{aligned}$$

So, we found the formula

$$\int_a^b f(x)dx = (b-a) f\Big(\frac{a+b}{2}\Big) + R(f), \tag{3.4}$$

called the **rectangle rule**, an *open* Newton-Cotes formula, having degree of precision $d = 1$, which is the *maximum* possible for a formula with a single node ($m = 0$).

We compute the remainder by

$$R(f) = \frac{f''(\xi)}{2!}\int_a^b \left(x - \frac{a+b}{2}\right)^2 dx = \frac{(b-a)^3}{24} f''(\xi),\ \xi \in (a,b). \tag{3.5}$$

Let us see a geometrical interpretation of this formula. Recall that, if $f(x) \geq 0$ for $x \in [a,b]$, the definite integral in (3.4) represents the area of the region that lies below the graph of $f(x)$, above the Ox axis and between the lines $x = a$ and $x = b$. This area is approximated by the area of the *rectangle* with base $b - a$ and height $f\left(\frac{a+b}{2}\right)$ (see Figure 1). Hence, the other name of the method.

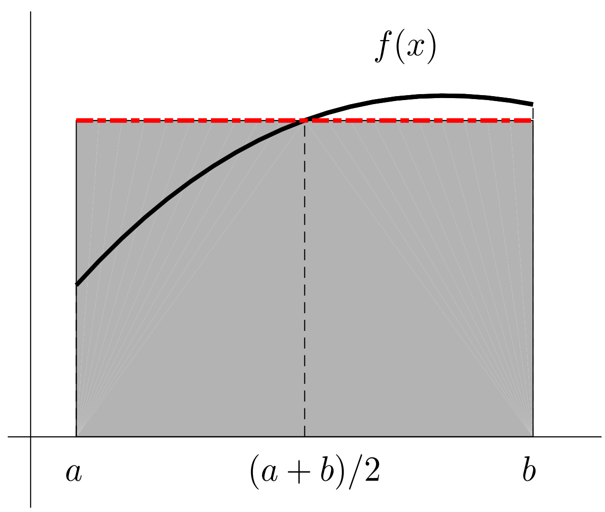

Fig. 1: Geometrical illustration of the rectangle rule

Remark 3.4. The rectangle rule (3.4) can also be obtained using the *method of undetermined coefficients*. We seek a quadrature formula with one node, i.e., of the form

$$\int_a^b f(x)dx = A_0 f(x_0) + R(f).$$

Then impose conditions (3.2) and go as far as possible.

Solution. First, we want $R(e_0) = 0$, which means

$$\int_a^b e_0(x)dx \;=\; A_0 e_0(x_0), \;\text{ i.e.,} \int_a^b dx \;=\; A_0.$$

We get the first equation, $A_0 = b - a$.
Then, from $R(e_1) = 0$, we obtain

$$\int_a^b e_1(x)dx \;=\; A_0 e_1(x_0), \;\text{ i.e.,} \int_a^b x dx \;=\; A_0 x_0,$$

so, the second equation is $A_0 x_0 = \dfrac{b^2 - a^2}{2}$. The two equations have the solution

$$\begin{aligned} A_0 &= b - a, \\ x_0 &= \frac{a+b}{2}. \end{aligned}$$

Can we go further? Let's check.

$$\begin{aligned} R(e_2) &= \int_a^b e_2(x)dx - (b-a)e_2\left(\frac{a+b}{2}\right) = \int_a^b x^2 dx - (b-a)\left(\frac{a+b}{2}\right)^2 \\ &= \frac{b^3 - a^3}{3} - (b-a)\,\frac{(a+b)^2}{4} = \frac{(b-a)^3}{12} \neq 0, \end{aligned}$$

so the degree of precision is $d = 1$. From here, we can obtain the expression of the remainder (3.5) using **Peano's theorem**. Let us recall this important result and see how it is used for quadratures formulas. For a numerical integration formula

$$\int_a^b f(x)\, dx \;=\; Q(f) + R(f),$$

with **degree of precision** $d = n$, assuming $f \in C^{n+1}[a, b]$, the remainder has the form

$$R(f) \;=\; \int_a^b K_n(t) f^{(n+1)}(t)\, dt,$$

with

$$
\begin{aligned}
K_n(t) &= \frac{1}{n!} R_n\big((x-t)_+^n\big) = \frac{1}{n!}\Big[\int\limits_a^b (x-t)_+^n \, dx - Q\big((x-t)_+^n\big)\Big] \\
&= \frac{1}{n!}\Big[\frac{1}{n+1}(x-t)_+^{n+1}\Big|_{x=a}^{x=b} - Q\big((x-t)_+^n\big)\Big] \\
&= \frac{1}{n!}\Big[\frac{(b-t)_+^{n+1} - (a-t)_+^{n+1}}{n+1} - Q\big((x-t)_+^n\big)\Big].
\end{aligned}
$$

If K_n has constant sign on $[a,b]$, then

$$
R(f) = \frac{1}{(n+1)!} f^{(n+1)}(\xi) R\big(e_{n+1}\big), \; \xi \in (a,b).
$$

So, for the midpoint formula

$$
\int\limits_a^b f(x)dx = (b-a) f\Big(\frac{a+b}{2}\Big) + R(f),
$$

with degree of precision $d=1$, we have

$$
R(f) = \int\limits_a^b K_1(t) f''(t) \, dt,
$$

with

$$
\begin{aligned}
K_1(t) &= \frac{1}{1!} R\big((x-t)_+\big) = \int\limits_a^b (x-t)_+ \, dx - (b-a)\left(\frac{a+b}{2} - t\right)_+ \\
&= \frac{1}{2}\big[(b-t)_+^2 - (a-t)_+^2\big] - (b-a)\left(\frac{a+b}{2} - t\right)_+ .
\end{aligned}
$$

Now, since $t \in [a,b]$, it follows that $(b-t)_+ = b-t$ and $(a-t)_+ = 0$. The third term depends on the sign of $\dfrac{a+b}{2} - t$. So, we have two cases:

1. $\boldsymbol{a \le t \le \frac{a+b}{2}}$, when $\left(\frac{a+b}{2}-t\right)_+ = \frac{a+b}{2}-t$ and, hence,

$$\begin{aligned} K_1(t) &= \frac{1}{2}(b-t)^2 - (b-a)\left(\frac{a+b}{2}-t\right) = \frac{1}{2}b^2 - bt + \frac{1}{2}t^2 - \frac{1}{2}(b^2-a^2) + bt - at \\ &= \frac{1}{2}t^2 - at + \frac{1}{2}a^2 = \frac{1}{2}(t-a)^2 \ge 0; \end{aligned}$$

2. $\boldsymbol{\frac{a+b}{2} < t \le b}$, when $\left(\frac{a+b}{2}-t\right)_+ = 0$ and we have

$$K_1(t) = \frac{1}{2}(b-t)^2 \ge 0.$$

So, in both cases, K_1 has a constant sign over $[a,b]$, and thus, the remainder can be expressed as

$$R(f) = \frac{1}{2!}f''(\xi)R\big(e_2\big) = \frac{(b-a)^3}{24}f''(\xi),\ \xi \in (a,b),$$

as in (3.5).

■

To improve on the approximation of the integral, break the interval $[a,b]$ into n smaller subintervals determined by the equidistant nodes $x_i = a + ih, i = \overline{0,n}, h = (b-a)/n$, and apply the rectangle rule (3.4) on each subinterval, i.e.,

$$\int_{x_i}^{x_{i+1}} f(x)dx = hf\Big(\frac{x_i+x_{i+1}}{2}\Big) + \frac{h^3}{24}f''(\xi_i),\ \xi_i \in [x_i,x_{i+1}].$$

We have

$$\int_a^b f(x)dx = \sum_{i=0}^{n-1}\int_{x_i}^{x_{i+1}} f(x)dx = h\sum_{i=0}^{n-1} f\Big(\frac{x_i+x_{i+1}}{2}\Big) + \frac{h^3}{24}\sum_{i=0}^{n-1} f''(\xi_i),\ \xi_i \in [x_i,x_{i+1}].$$

Using a mean value formula for the continuous function f'',

$$f''(\xi) = \frac{f''(\xi_0) + \cdots + f''(\xi_{n-1})}{n},\ \xi \in (a,b),$$

we get

$$\int_a^b f(x)dx = h\sum_{i=0}^{n-1} f\Big(a+\big(i+\frac{1}{2}\big)h\Big) + \frac{h^2(b-a)}{24}f''(\xi),\ \xi\in(a,b), \tag{3.6}$$

called the **composite (repeated) rectangle (midpoint) formula**.

Trapezoidal Rule

We proceed similarly, approximating the integrand by the Lagrange interpolation polynomial with 2 nodes, $x_0 = a, x_1 = b$, the endpoints of the interval. If f is twice continuously differentiable on (a, b), we have

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

Integrating, after doing all the computations, we get

$$\int_a^b f(x)dx = \frac{b-a}{2}\Big(f(a)+f(b)\Big) - \frac{(b-a)^3}{12}f''(\xi),\ \xi\in(a,b), \tag{3.7}$$

called the **trapezoidal (or trapezium) rule**, a *closed* Newton-Cotes formula. Again, the name comes from the geometrical interpretation (see Figure 2), where the area of the region that lies between the graph of f, the $x-$axis and the lines $x = a$ and $x = b$, is approximated by the area of the trapezoid with bases $f(a), f(b)$ and height $b - a$.

Since this rule is derived from Lagrange interpolation with two nodes (the degree of the interpolation polynomial being 1), we know that its degree of precision is *at least* $d = 1$ (without checking $R(e_0) = R(e_1) = 0$). Let us check if $d > 1$.

$$R(e_2) = \int_a^b x^2dx - \frac{b-a}{2}\big(a^2+b^2\big) = \frac{1}{3}\big(b^3-a^3\big) - \frac{b-a}{2}\big(a^2+b^2\big) = -\frac{(b-a)^3}{6} \neq 0.$$

Thus, the degree of precision is $d = 1$.

Now, just as we did with the rectangle rule, we divide the interval $[a, b]$ into n subintervals

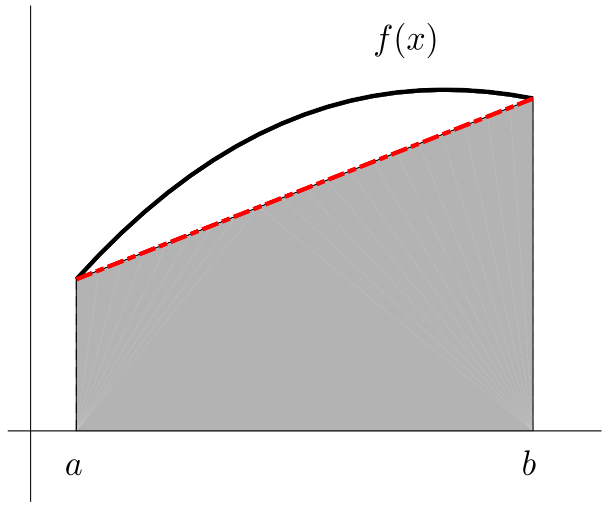

Fig. 2: Geometrical illustration of the trapezoidal rule

$[x_i, x_{i+1}],\ x_i = a + ih, i = \overline{0, n}$, of length $h = \dfrac{b-a}{n}$. We have

$$\int_a^b f(x)dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)dx = \frac{h}{2} \sum_{i=0}^{n-1} \Big(f(x_i) + f(x_{i+1}) \Big) - \frac{h^3}{12} \sum_{i=0}^{n-1} f''(\xi_i),\ \xi_i \in [x_i, x_{i+1}]$$

Using again the mean value theorem and denoting by $f_i = f(x_i)$, we get the **composite (repeated) trapezoidal (trapezium) rule**,

$$\int_a^b f(x)dx = \frac{h}{2} \Big[f(a) + 2\big(f_1 + \cdots + f_{n-1}\big) + f(b) \Big] - \frac{h^2(b-a)}{12} f''(\xi),\ \xi \in (a, b). \quad (3.8)$$

Remark 3.5. Obviously, for larger n, we get increasingly accurate approximations of the definite integral. But which sequence of values of n should be used? If n is doubled repeatedly, $n \to 2n$, then the function values used in each approximation (3.8) will include all of the earlier function values used in the preceding approximation. Thus, the *doubling* of n will ensure that all previously computed information is used in the new calculation, making the trapezoidal rule less expensive than it would be otherwise.

Simpson's Rule

For this formula, we consider Hermite interpolation at the nodes $x_0 = a, x_1 = \dfrac{a+b}{2}$, *double* and $x_2 = b$. Then the corresponding Hermite interpolation polynomial has degree 3 and is of the form

$$\begin{aligned} H_3(x) &= f(x_0) + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_1](x - x_0)(x - x_1) + \\ &+ f[x_0, x_1, x_1, x_2](x - x_0)(x - x_1)^2. \end{aligned}$$

If f has continuous derivatives of order 4 on $[a, b]$, the error of the approximation can be written as

$$R_3(x) = \frac{(x - x_0)(x - x_1)^2(x - x_2)}{4!} f^{(4)}(\xi),\ \xi \in (a, b).$$

Integrating on $[a, b]$ the relation $f(x) = H_3(x) + R_3(x)$, we get a new closed Newton-Cotes formula,

$$\int_a^b f(x)dx = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] - \frac{(b-a)^5}{2880} f^{(4)}(\xi),\ \xi \in (a, b), \tag{3.9}$$

called the **(Cavalieri–) Simpson rule**. Its degree of precision is $d = 3$.

Dividing the interval $[a, b]$ into an *even* number $n = 2m$ of subintervals of length $h = \dfrac{b-a}{2m}$, and denoting by $x_i = a + ih, f_i = f(x_i), i = \overline{0, 2m}$, we have

$$\begin{aligned} \int_a^b f(x)dx &= \sum_{i=1}^{m} \int_{x_{2i-2}}^{x_{2i}} f(x)dx \\ &= \sum_{i=1}^{m} \left[\frac{h}{3}\Big(f_{2i-2} + 4f_{2i-1} + f_{2i}\Big) - \frac{h^5}{90} f^{(4)}(\xi_i)\right],\ \xi_i \in [x_{2i-2}, x_{2i}]. \end{aligned}$$

By the mean value theorem, we get the **composite (repeated) Simpson's rule**

$$\begin{aligned} \int_a^b f(x)dx &= \frac{h}{3}\left[f(a) + 4\sum_{i=1}^{m} f_{2i-1} + 2\sum_{i=1}^{m-1} f_{2i} + f(b)\right] \\ &- \frac{h^4(b-a)}{180} f^{(4)}(\xi),\ \xi \in (a, b). \end{aligned} \tag{3.10}$$

Remark 3.6.

1. The trapezoidal and Simpson's rules can also be derived using the method of undetermined coefficients for a two-point and three-point, respectively, quadrature formula.

2. Simpson's formula can be derived by considering interpolation with 3 *simple* nodes, so a polynomial of degree 2. We get the same coefficients, but the integral of the remainder will be zero. This is why Hermite interpolation was used instead.

3. These are three of the simplest quadrature formulas. The rectangle and trapezoidal rules are comparable precision-wise ($O(h^2)$) and also from the computational cost point of view (number of flops per iteration). The trapezoidal rule is usually preferred when the number of nodes is doubled at each iteration (see Remark 3.5). Simpson's rule is superior in precision ($O(h^4)$), but it also incurs a higher computational load.

Example 3.7. Approximate the integral

$$\int_0^1 \frac{1}{1+x}dx$$

using the three methods above.

Solution. The exact value of the integral is

$$\int_0^1 \frac{1}{1+x}dx \;=\; \ln(1+x)\Big|_0^1 \;=\; \ln 2 \;=\; 0.693147180559945.$$

By the rectangle rule, we have the approximation

$$\int_0^1 \frac{1}{1+x}dx \;\approx\; 1\cdot f\Big(\frac{1}{2}\Big) \;=\; \frac{2}{3} \;=\; 0.6667,$$

with error $E_1 \;=\; 0.0265$. Using the trapezoidal rule, we obtain

$$\int_0^1 \frac{1}{1+x}dx \;\approx\; \frac{1}{2}\big(f(0)+f(1)\big) \;=\; \frac{3}{4} \;=\; 0.75,$$

with error $E_2 = -0.0569$. Finally, with Simpson's rule, we get

$$\int_0^1 \frac{1}{1+x}dx \approx \frac{1}{6}\left[f(0)+4f\left(\frac{1}{2}\right)+f(1)\right] = \frac{25}{36} = 0.6944,$$

with approximation error $E_3 = -0.0013$.

■

Example 3.8. Let us approximate

$$\int_0^1 e^{-x^2}dx = 0.746824132812427,$$

with the composite trapezoidal and Simpson's rules.

Solution. The approximation errors (as well as the ratios of successive approximations) for the two methods are given in Table 2, for various values of n. These confirm the higher rate of convergence, $O(h^4)$, of Simpson's repeated method over the composite trapezoidal rule.

	Composite Trapezoidal		Repeated Simpson	
n	Error	Ratio	Error	Ratio
2	$1.55e-2$		$3.56e-4$	
4	$3.84e-3$	4.02	$3.12e-5$	11.4
8	$9.59e-4$	4.01	$1.99e-6$	15.7
16	$2.40e-4$	4.00	$1.25e-7$	15.9
32	$5.99e-5$	4.00	$7.79e-9$	16.0
64	$1.50e-5$	4.00	$4.87e-10$	16.0
128	$3.74e-6$	4.00	$3.04e-11$	16.0

Table 2: Example 3.8

■

Let us see another example of obtaining a quadrature formula two ways.

Example 3.9. Consider a quadrature formula of the type

$$\int_{-1}^{1} f(x)\,dx = Af'(-1)+Bf(1)+R(f).$$

a) Find A and B such that the formula has the maximum degree of exactness possible.

b) Let $B_1 f$ be the Birkhoff polynomial interpolating f, given $f'(-1)$ and $f(1)$. Compute $\int\limits_{-1}^{1} (B_1 f)(x)\, dx$ and compare it to the formula found in **a)**.

c) Express the remainder $R(f)$ in the form

$$R(f) \;=\; const \cdot f''(\xi),\; \xi \in (-1, 1).$$

Solution.

a) We set $R(e_k) = 0, e_k(x) = x^k$ and go as far as possible.

$$\begin{aligned} R(e_0) &= 2 - \Big[A \cdot 0 + B \cdot 1\Big] \;=\; 2 - B \;=\; 0, \\ R(e_1) &= 0 - \Big[A \cdot 1 + B \cdot 1\Big] \;=\; -A - B \;=\; 0. \end{aligned}$$

From these two equations, we get $A = -2$ and $B = 2$. Check further:

$$R(e_2) \;=\; \frac{2}{3} - \Big[-2 \cdot (-2) + 2 \cdot 1\Big] \;=\; \frac{2}{3} - 6 \;=\; -\frac{16}{3} \;\neq\; 0,$$

so the maximum degree of precision possible is $d = 1$ and the quadrature formula is

$$\int\limits_{-1}^{1} f(x) \;=\; 2\big(-f'(1) + f(1)\big) + R(f).$$

b) For Birkhoff interpolation, we have the nodes $x_0 = -1, x_1 = 1$ and $I_0 = \{1\}, I_1 = \{0\}$. Then the degree of the polynomial is $n = 1 + 1 - 1 = 1$. The polynomial

$$B_1 f(x) \;=\; ax + b$$

must satisfy the interpolation conditions

$$\left\{ \begin{aligned} (B_1 f)'(-1) &= f'(-1) \\ (B_1 f)(1) &= f(1) \end{aligned} \right. \iff \left\{ \begin{aligned} a \quad &= f'(-1) \\ a + b &= f(1) \end{aligned} \right. \iff \left\{ \begin{aligned} a &= f'(-1) \\ b &= f(1) - f'(-1) \end{aligned} \right. .$$

So, we have

$$\begin{aligned} f(x) &= (B_1 f)(x) + (R_1 f)(x) \\ &= x f'(-1) + \big(f(1) - f'(-1)\big) + (R_1 f)(x) \\ &= (x-1) f'(-1) + f(1) + (R_1 f)(x) \\ &= b_{01}(x) f'(-1) + b_{10}(x) f(1) + (R_1 f)(x). \end{aligned}$$

Integrating, we get

$$\begin{aligned} \int_{-1}^{1} f(x)\,dx &= \int_{-1}^{1} (B_1 f)(x)\,dx + R(f) \\ &= f'(-1) \int_{-1}^{1} (x-1)\,dx + f(1) \int_{-1}^{1} dx + R(f) \\ &= -2f'(-1) + 2f(1) + R(f), \end{aligned}$$

the same quadrature formula as before.

c) The degree of precision is $d = 1$. Then,

$$R(f) = \int_{-1}^{1} K_1(t) f''(t)\,dt,$$

with

$$\begin{aligned} K_1(t) = R\big((x-t)_+\big) &= \int_{-1}^{1} (x-t)_+\,dx - 2\Big[-\frac{\partial (x-t)_+}{\partial x}\Big|_{x=-1} + (1-t)_+\Big] \\ &= \frac{1}{2}(x-t)_+^2\Big|_{x=-1}^{x=1} - 2\Big[-1 + (1-t)_+\Big] \\ &= \frac{1}{2}\Big((1-t)_+^2 - (-1-t)_+^2\Big) + 2 - 2(1-t)_+. \end{aligned}$$

Since $t \in [-1, 1]$, $(1-t)_+ = 1-t$, $(-1-t)_+ = 0$ and further we have

$$K_1(t) \;=\; \frac{1}{2}(1-t)^2 + 2 - 2(1-t) \;=\; \frac{1}{2}(1-t)^2 + 2t \;=\; \frac{1}{2}(1+t)^2 \;\geq\; 0.$$

So,

$$R(f) \;=\; \frac{1}{2}f''(\xi)R(e_2) \;=\; \frac{1}{2}\left(-\frac{16}{3}\right)f''(\xi) \;=\; -\frac{8}{3}f''(\xi),\; \xi \in (-1, 1).$$

Alternatively, we can find the remainder in the Birkhoff interpolation formula, using Peano's Theorem:

$$(R_1 f)(x) \;=\; \frac{(x-1)(x+3)}{2}f''(\xi),\; \xi \in (-1, 1).$$

(try it, it's a good exercise). Then, integrating, we get

$$R(f) \;=\; \int\limits_{-1}^{1}(R_1 f)(x)\,dx \;=\; -\frac{8}{3}f''(\xi),\; \xi \in (-1, 1),$$

same as before.

■

3.2 Adaptive Quadratures

As seen so far, the errors in numerical integration methods depend not only on the size of the interval, but also on values of certain higher order derivatives of the function to be integrated. Newton-Cotes methods (including the three simple ones, that use low degree polynomial interpolation) work well for smooth integrands (even with a small number of nodes), but perform poorly for functions having large values of higher order derivatives – especially for functions having large oscillations on some subintervals or on the whole interval. As a simple example, consider

$$\int\limits_{0}^{1}\sqrt{x}\,dx \;=\; \frac{2}{3}.$$

This integrand has infinite derivative at $x = 0$, but is smooth at points close to $x = 1$.

Generally, numerical integration schemes use evenly spaced nodes. When the function to be integrated has a singularity at some point $\alpha \in [a, b]$, this requires many nodes in the vicinity of that point, to reduce the errors caused by the chaotic behaviour of the function in that neighborhood. But this implies that many more nodes (more than necessary) are used throughout the *entire* interval of integration, increasing (unnecessarily) the computational cost of the method. Ideally, we want to use small subintervals where the derivatives are large, and larger subintervals where the derivatives are small and well-behaved.

A method that does this systematically is called **adaptive quadrature**. The general approach in an adaptive quadrature is to use two different methods on each subinterval, compare the results, and divide the interval when the differences are large. The structure of such an algorithm would be "Divide and conquer".

In Algorithm 3.1 we present an example of a general structure for a recursive adaptive quadrature. The parameter "met" is a function that implements a composite quadrature rule, such as the trapezoidal or Simpson's rule, and m is the number of subintervals.

Unlike other methods, that decide what amount of work is needed to achieve a desired precision, an adaptive quadrature computes only as much as is necessary.

Algorithm 3.1. [Adaptive quadrature]

function $I = adquad(f, a, b, \varepsilon, met, m)$
    $I1 = met(f, a, b, m)$;
    $I2 = met(f, a, b, 2m)$;
    if $|I1 - I2| < \varepsilon$ % success
        $I = I2$;
        return
    else % recursive subdivision
        $I = adquad(f, a, \frac{a+b}{2}, \varepsilon, met, m) + adquad(f, \frac{a+b}{2}, b, \varepsilon, met, m)$;
    end
end