Chapter 3. 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*.

Definition 1.5. *If $\mathbb{P}_d \subset X$, the number $d \in \mathbb{N}$ satisfying the property $\ker R = \mathbb{P}_d$ is called **degree of precision (exactness)** of the approximation formula* (1.1).

Remark 1.6. Since R is a linear functional, the following are equivalent:

$$\ker R = \mathbb{P}_d \iff \begin{cases} R(e_k) = 0, \; k = 0, 1, \ldots, d, \\ R(e_{d+1}) \neq 0, \end{cases} \tag{1.2}$$

with $e_k(x) = x^k$.

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 using the relations from (1.2).

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

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

Example 2.1. Use $D_h f(x)$ (formula (2.1)) to approximate the derivative of $f(x) = \cos x$ at $x = \pi/6$. Study the error of the approximation.

Solution. The exact value is

$$f'\Big(\frac{\pi}{6}\Big) \;=\; -\sin\frac{\pi}{6} \;=\; -\frac{1}{2}.$$

By (2.2), 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,

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

Table 1 contains the approximation results for various values of h. Indeed, the value of $D_h f$ is approaching -0.5. Moreover, looking at the errors, we see that when h is halved, the error is almost halved (see the ratio column). This confirms the fact that the error is proportional to h (relation (2.2)). ■

h	$D_h f$	Error	Ratio
0.1	-0.54243	0.04243	
0.05	-0.52144	0.02144	1.98
0.025	-0.51077	0.01077	1.99
0.0125	-0.50540	0.00540	1.99
0.00625	-0.50270	0.00270	2.00
0.003125	-0.50135	0.00135	2.00

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

2.1 Interpolation Method

Consider Newton's interpolation formula

$$f(x) = N_n f(x) + R_n f(x), \tag{2.5}$$

with

$$\begin{aligned} N_n f(x) &= f(x_0) + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) \\ &+ f[x_0, x_1, x_2, x_3](x - x_0)(x - x_1)(x - x_2) + \ldots \\ &+ f[x_0, \ldots, x_n](x - x_0) \ldots (x - x_{n-1}), \\ R_n f(x) &= f[x, x_0, \ldots, x_n](x - x_0) \ldots (x - x_n). \end{aligned}$$

Taking the first derivative in (2.5), we get

$$\begin{aligned} f'(x) &= f[x_0, x_1] + f[x_0, x_1, x_2](x - x_1 + x - x_0) + \dots \\ &+ f[x_0, \dots, x_n]\Big((x - x_0)\dots(x - x_{n-1})\Big)' \\ &+ (R_n f)'(x). \end{aligned} \tag{2.6}$$

Assuming that f has $n+1$ continuous derivatives on a suitable interval, for the remainder, we have

$$\begin{aligned} (R_n f)'(x) &= \frac{f^{(n+1)}(\xi_x)}{(n+1)!}\Big((x - x_0)\dots(x - x_n)\Big)' \\ &= \frac{f^{(n+1)}(\xi_x)}{(n+1)!}\sum_{i=0}^{n}(x - x_0)\dots(x - x_{i-1})(x - x_{i+1})\dots(x - x_n), \end{aligned} \tag{2.7}$$

where ξ_x lies in the smallest interval containing $x_0, \dots, x_n$ and x.

Similarly, differentiating twice, we get

$$\begin{aligned} f''(x) &= 2f[x_0, x_1, x_2] + f[x_0, x_1, x_2, x_3]\Big((x - x_0)(x - x_1)(x - x_2)\Big)'' + \dots \\ &+ f[x_0, \dots, x_n]f[x_0, \dots, x_n]\Big((x - x_0)\dots(x - x_{n-1})\Big)'' \\ &+ (R_n f)''(x). \end{aligned} \tag{2.8}$$

Let us consider a few cases:

- For $n = 1$ and the nodes $x_0 = x, x_1 = x + h$, from (2.6) we get the numerical differentiation formula

  $$f'(x) \approx f[x, x+h] = \frac{f(x+h) - f(x)}{h},$$

  and for the remainder, by (2.7),

  $$(R_1 f)'(x) = \frac{f''(\xi_x)}{2!}(2x - x_0 - x_1) = -\frac{h}{2}f''(\xi_x),\ x \leq \xi_x \leq x + h,$$

  so, we find again the forward difference numerical derivative.

- In a similar manner, for $n = 1$ and the nodes $x_0 = x - h, x_1 = x$, we obtain again the backward difference numerical derivative.

- An interesting case is $n = 2$, with the nodes $x_0 = x - h, x_1 = x, x_2 = x + h$. By (2.6),

$$\begin{aligned} f'(x) &\approx f[x_0, x_1] + f[x_0, x_1, x_2](x - x_1 + x - x_0) \\ &= \frac{f(x+h) + f(x-h)}{2h} \equiv \widehat{D}_h f(x), \end{aligned} \tag{2.9}$$

known as the *central difference numerical derivative formula*. In this case, for the remainder, we get from (2.7),

$$\begin{aligned} (R_2 f)'(x) &= \frac{f'''(\xi_x)}{3!}(x - x_0)(x - x_2) \\ &= -\frac{h^2}{6} f'''(\xi_x), \; x - h \le \xi_x \le x + h. \end{aligned} \tag{2.10}$$

This says that for small values of h, the formula (2.9) should be more accurate than the earlier approximations, because the error term of (2.10) decreases more rapidly with h.

Example 2.2. Consider again $f(x) = \cos x$. Let us approximate $f'(\pi/6)$ using (2.9).

Solution. The results of the approximation are given in Table 2, and they confirm the rate of convergence of $O(h^2)$ given in (2.10).

h	$\widehat{D}_h f$	Error	Ratio
0.1	-0.49916708	$-8.329e-4$	
0.05	-0.49979169	$-2.083e-4$	4.00
0.025	-0.49994792	$-5.208e-5$	4.00
0.0125	-0.49998698	$-1.302e-5$	4.00
0.00625	-0.49999674	$-3.255e-6$	4.00

Table 2: Example 2.2, $f(x) = \cos x$

■

This procedure can be carried on, to approximate higher order derivatives.

2.2 Method of Undetermined Coefficients

In general, the method of undetermined coefficients is used when we seek an approximation method of a specific form, using specific values. We illustrate it by finding an approximation formula for the second derivative, of the form

$$f''(x) \approx D_h^{(2)} f(x) \equiv Af(x+h) + Bf(x) + Cf(x-h),\ h > 0. \tag{2.11}$$

We determine the unknown coefficients A, B and C the following way: replace $f(x+h)$ and $f(x-h)$ by their Taylor polynomials,

$$\begin{aligned} f(x+h) &\approx f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(x), \\ f(x-h) &\approx f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(x). \end{aligned}$$

Including more terms would give higher powers of h and for small values of h, these additional terms should be much smaller than the terms already included above (so, negligible). Substituting these approximations into the formula for $D_h^{(2)} f(x)$ and collecting together common powers of h give us

$$\begin{aligned} D_h^{(2)} f(x) &\approx (A+B+C)f(x) + h(A-C)f'(x) + \frac{h^2}{2}(A+C)f''(x) \\ &+ \frac{h^3}{6}(A-C)f'''(x) + \frac{h^4}{24}(A+C)f^{(4)}(x). \end{aligned} \tag{2.12}$$

To have

$$D_h^{(2)} f(x) \approx f''(x),$$

for arbitrary functions f, it is necessary to require that the coefficients of f and f' be 0, while the coefficient of f'' should be 1. We obtain the system

$$\begin{cases} A+B+C = 0 \\ h(A-C) = 0 \\ \dfrac{h^2}{2}(A+C) = 1 \end{cases}$$

with solution

$$A = C = \frac{1}{h^2},\ B = -\frac{2}{h^2}, \tag{2.13}$$

hence, the formula

$$D_h^{(2)} f(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}. \tag{2.14}$$

To determine the error, notice that (with these values of the coefficients) in (2.12) we get

$$D_h^{(2)} f(x) \;\approx\; f''(x) + \frac{h^2}{12} f^{(4)}(x).$$

Thus, we have the error

$$(RD_h^{(2)} f)(x) \;=\; f''(x) - D_h^{(2)} f(x) \;\approx\; -\frac{h^2}{12} f^{(4)}(x). \tag{2.15}$$

Example 2.3. For $f(x) = \cos x$, approximate $f''(\pi/6)$ using formula (2.14).

Solution. The exact value is

$$f''\left(\frac{\pi}{6}\right) \;=\; -\cos\frac{\pi}{6} \;=\; -\frac{\sqrt{3}}{2} \;=\; -0.8660.$$

The results of the approximation are shown in Table 3. Note that the ratio column is consistent with the error formula (2.15), i.e. a rate of convergence of $O(h^2)$.

h	$D_h^{(2)} f$	Error	Ratio
0.5	-0.84813289	$-1.789e-2$	
0.25	-0.86152424	$-4.501e-3$	3.97
0.125	-0.86489835	$-1.127e-3$	3.99
0.0625	-0.86574353	$-2.819e-4$	4.00
0.03125	-0.86595493	$-7.048e-5$	4.00

Table 3: Example 2.3, $f(x) = \cos x$

■

Remark 2.4.

1. Alternately, the coefficients A, B and C could have been found by imposing relations $R(e_k) = 0, k = 0, 1, \ldots, d$ from (1.2). In this case, the remainder could be computed using Peano's Theorem.

2. Also, the numerical differentiation formula (2.14) (and its error) can be derived with the interpolation method, using (2.8).

3. 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

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

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*

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

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****.*

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*** *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

$$R(e_j) = 0,\ j=0,1,\dots,d,\ R(e_{d+1})\neq 0. \qquad (3.2)$$

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

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

$$d_{\max} \;=\; 2m+1.$$

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

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

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

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

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.

Remark 3.4. The rectangle rule (3.4) can also be obtained using the method of undetermined coef-

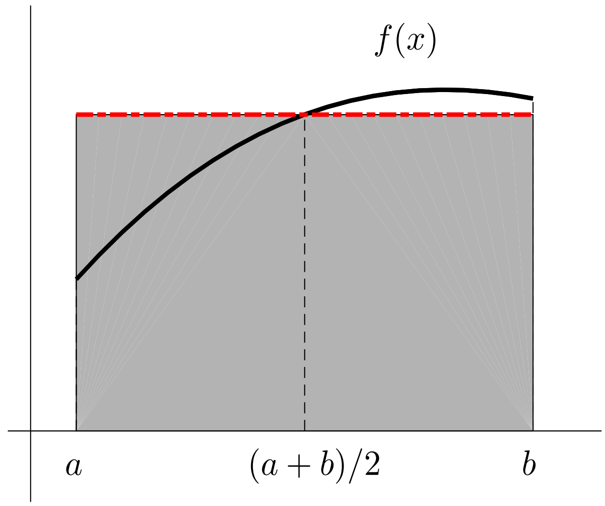

Fig. 1: Geometrical illustration of the rectangle rule

ficients, starting with

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

and imposing conditions (3.2). From $R(e_0) = 0$, we get $A_0 = b - a$, and in order to have $R(e_1) = 0$, the node x_0 must be the midpoint of the interval, $x_0 = \dfrac{a+b}{2}$.

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

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

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

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

called the **trapezoidal 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 $d > 1$.

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

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

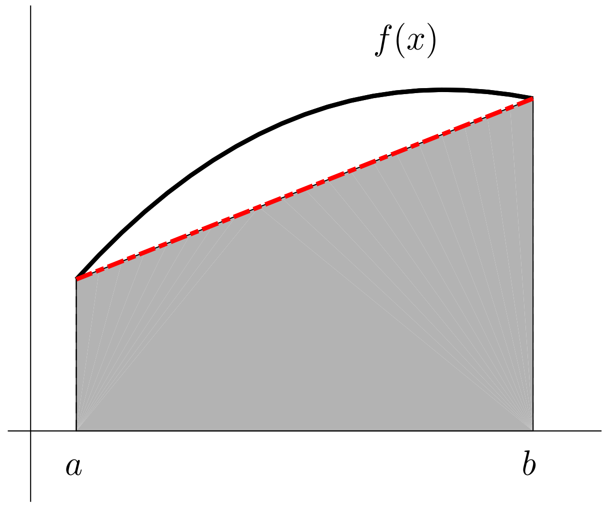

Fig. 2: Geometrical illustration of the trapezoidal rule

Now, just as we did with the rectangle rule, we divide the interval $[a,b]$ into n subintervals $[x_i, x_{i+1}],\ x_i = a + ih, i = \overline{0,n}$, 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 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,

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

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**

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

Remark 3.6.
1. 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.
2. 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 ratio of successive approximations) for the two methods are given in Table 4, 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 4: Example 3.8

■