and determining the percentage of anomalous larvae p_i found in each of them. To measure an environment's toxicity T_x, the test is repeated with a bioassay determining again the percentages p_x of anomalous larvae. Write a program to determine the degree of toxicity T_x by interpolating the data measured in the laboratory with a generic Lagrange polynomial of degree $N-1$. The input consists of a file containing two columns which represent, respectively, the values p_i measured in the laboratory for the corresponding T_i and the values of p_x measured in the latter test. The output is the value of T_x. Graphically compare the obtained Lagrange polynomial with the experimental data.

Hands on 4 - Interpolating functions

Euler's Γ function, used to define many statistical functions, is defined by an integral, whose primitive is not known analytically. On the other hand, evaluating this integral with numerical methods is a particularly burdensome task in terms of CPU time. The function, defined as

$$\Gamma(x) = \int_0^\infty u^{x-1} e^{-u} du \,,$$

has the following property: if x is a positive integer, $\Gamma(x) = (x-1)!$. Thus, one way to obtain the values is by interpolating it using a finite number of finite points $x_1, \ldots, x_n$ with x_i integer. Write a program estimating the values of the function $\Gamma(x)$ by means of Lagrange polynomials of different degrees (try both with polynomials of low degree, such as 1, 2 or 3, and degrees greater than 10). Compare the obtained values with the ones listed in mathematics textbooks. In particular, we have that $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$, $\Gamma\left(\frac{3}{2}\right) = \frac{1}{2}\sqrt{\pi}$ and $\Gamma\left(\frac{5}{2}\right) = \frac{3}{4}\sqrt{\pi}$.

8.2 Numerical integration

Problems of a scientific nature often require we evaluate defined integrals. In this section we study the methods to compute integrals of the type

$$I = \int_a^b f(x)\, dx \,. \tag{8.16}$$

Of course, if we know the antiderivative $F(x)$ of $f(x)$, we can always write a function returning its value and compute the definite integral as a difference

$$I = F(b) - F(a) \ .$$

Unfortunately, the antiderivative of the integrand is not always known analytically. This is the case, for example, for numerous, frequently used probability distributions, from the Gaussian distribution to the χ^2 and the Student's t-distribution. In other cases it might be necessary to create a generic integrating function, independent of the particular form of the function f, to include it, e.g., in a mathematical library. In these cases, the integral I can only be approximated to its true value. This is referred to as numerical integration.

Before we show the methods for numerical integration, we observe that due to the additive property of integrals, setting $c_0 = a$, $c_M = b$, we can write

$$I = \int_a^b f(x)\, dx = \sum_{i=0}^{M-1} \int_{c_i}^{c_{i+1}} f(x)\, dx = \sum_{i=0}^{M-1} I_i \, ,$$

with $c_k \in [a, b]\ \forall k$. Therefore, we can limit ourselves to select one single term of the summation by choosing an interval which can be, within the limits of the computer architecture, as small as we want.

In these cases, the most natural operation is to substitute the integrand with another function. The latter should approximate the integrand well and be a function of which we know the antiderivative. Such a function exists, namely the Lagrange polynomial. Computing the integral I thus is equivalent to the evaluation of the integral of a polynomial,

$$I_i = \int_{c_i}^{c_{i+1}} f(x)\, dx \simeq I_i^{(n)} \equiv \int_{c_i}^{c_{i+1}} L_{n-1}(x)\, dx \, . \tag{8.17}$$

The expression (8.17) represents an entire family of different integration methods, depending on the degree of the Lagrange polynomial. The remainder of the Lagrange polynomial, given by equation (8.15), allows us to evaluate the maximum error, or remainder, we make using such an approximation. For simplicity, we suppose all intervals composing $[a, b]$ have the same size $h = c_{i+1} - c_i$. Let us set

$$\delta_i^{(n)} = \left| I_i - I_i^{(n)} \right| \leq \int_{c_i}^{c_{i+1}} |\Delta_n| \ dx \, .$$

By substituting Δ_n with the right–hand member of the inequality of expression (8.15) and performing the following substitution

$$x = \frac{c_{i+1}+c_i}{2} + \frac{c_{i+1}-c_i}{2}t = \frac{c_{i+1}+c_i}{2} + \frac{h}{2}t \qquad \Rightarrow \qquad dx = \frac{h}{2}\,dt\,,$$

we have

$$\delta_i^{(n)} \leq \left|\sup_{\xi\in[c_i,c_{i+1}]} f^{(n)}(\xi)\right| \frac{1}{n!}\int_{-1}^{+1}\prod_{j=1}^{n}|t-t_j|\left(\frac{h}{2}\right)^{n+1} dt = A_i^{(n)}(f)\left(\frac{h}{2}\right)^{n+1} D_n\,,$$

where $A_i^{(n)}(f)$ represents the maximum value of the function's nth derivative in the interval and

$$D_n \equiv \frac{1}{n!}\int_{-1}^{+1}\prod_{j=1}^{n}|t-t_j|\,dt\,.$$

Finally, summing the various contributions and considering that $Mh = b-a$, we obtain the error δ on the integral, given by equation (8.16), is

$$\delta^{(n)} = \sum_{i=0}^{M-1}\delta_i^{(n)} = \left(\frac{h}{2}\right)^{n+1} D_n \sum_{i=0}^{M-1} A_i^{(n)}(f) \leq \frac{A_n(f)D_n}{2^{n+1}}h^n(b-a) = = \frac{A_n(f)D_n}{2^{n+1}}\frac{(b-a)^{n+1}}{M^n}\,, \quad (8.18)$$

where

$$A_n(f) \equiv \max_i A_i^{(n)} = \left|\sup_{\xi\in[a,b]} f^{(n)}(\xi)\right|\,.$$

As expected, this relation tells us that the error with which we can estimate the value of the integral decreases as the size of the single integration interval h decreases (it decreases if the number M of points in which we divide the interval $[a,b]$ increases). Instead, for larger integration intervals the error may increase a lot.

8.2.1 *The rectangle rule*

If the integrand can be approximated with a constant C in the integration interval (i.e., if the integration interval is small enough such that we can consider $f(x)$ to be constant in that interval), we can write

$$\int_{c_i}^{c_{i+1}} f(x)\,dx \simeq I_i^{(1)} = C\,(c_{i+1} - c_i) = Ch\,, \tag{8.19}$$

where $C = f(\xi)$ and $\xi \in [c_i, c_{i+1}]$ is arbitrary. This corresponds to substituting the integrand with a Lagrange polynomial with degree 0 passing through the point $(\xi, f(\xi))$.

The relation (8.19) is called the rectangle rule[2] It takes this name because from a geometric point of view, calculating I_i is equivalent to calculating the area of a rectangle with base $h = (c_{i+1} - c_i)$ and height C (as shown in Fiigure 8.1). The remainder of this quadrature formula is easily derived using equation (8.18) with $n = 1$ and is

$$\delta^{(1)} \le \left| \sup_{\xi\in[a,b]} f'(\xi) \right| D_1 \frac{(b-a)^2}{4M} = \left| \sup_{\xi\in[a,b]} f'(\xi) \right| D_1 \frac{b-a}{4} h\,, \tag{8.20}$$

where D_1 may vary, depending on the choice of the point ξ, between 1 and 2. In general, this method is used when the function to be integrated is unknown, but its value is known in some points (for example, as a result of some measurement). Instead, when the function to be integrated is known, the midpoint method is used.

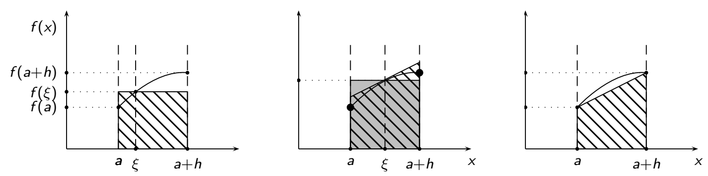

Fig. 8.1 From a geometric point of view, the rectangle rule corresponds to substituting the integral of the curve $f(x)$ with the outlined area in the figure on the left. Instead, the trapezoidal rule approximates the curve's integral with the area of the trapezoid shown in the rightmost figure. The midpoint method is shown in the figure in the middle. The area of the outlined trapezoid (with the oblique side tangent to the curve in ξ) is equal to the one of the gray rectangle (with one side passing through ξ).

[2]The formula (8.19) is also called Newton's quadrature formula. Indeed, Newton introduced this method to evaluate the area of the portion of the plane included between the horizontal axis and the curve described by the integrand, when differential calculus did not yet exist.

8.2.2 *The midpoint method*

The midpoint method is a special case of the rectangle rule. It consists in choosing for ξ the midpoint of the interval or, in terms of the variable t, $t_1 = 0$. The performance of the integration method can be improved exploiting the symmetry properties of the interpolating polynomial. If we choose ξ as the midpoint of the interval, $\xi = (c_{i+1} + c_i)/2$, it is easy to understand that the rectangle with base h and height $f(\xi)$ is equivalent to whichever trapezoid of height h, with the oblique side passing through $f(\xi)$. So, instead of approximating the function f with a constant, we approximate it with a straight line passing through the point

$$\left(\frac{c_i + c_{i+1}}{2}, f\left(\frac{c_i + c_{i+1}}{2}\right)\right) . \tag{8.21}$$

The quadrature formula remains the same, namely (8.19), but the error is smaller. Indeed, expanding the function $f(x)$ in series around the midpoint, we have that

$$f(x) \simeq f\left(\frac{c_i + c_{i+1}}{2}\right) + f'\left(\frac{c_i + c_{i+1}}{2}\right)\left(x - \frac{c_i + c_{i+1}}{2}\right) + \\ + \frac{1}{2}f"\left(\frac{c_i + c_{i+1}}{2}\right)\left(x - \frac{c_i + c_{i+1}}{2}\right)^2 + \dots$$

The first two terms of the series represent precisely a straight line passing through the point (8.21). Therefore, the error we made with this approximation is given by

$$\delta_i^{(1)} \le \left|\frac{1}{2}f"\left(\frac{c_i + c_{i+1}}{2}\right)\right| \int_{c_i}^{c_{i+1}} \left|\left(x - \frac{c_i + c_{i+1}}{2}\right)^2\right| dx = \\ = \frac{1}{24}\left|f"\left(\frac{c_i + c_{i+1}}{2}\right)\right| (c_{i+1} - c_i)^3 ,$$

from which we obtain that

$$\delta^{(1)} \le \frac{1}{24}\left|\sup_{\xi\in[a,b]} f"(\xi)\right| h^2(b-a) = \frac{1}{24}\left|\sup_{\xi\in[a,b]} f"(\xi)\right| \frac{(b-a)^3}{M^2} , \tag{8.22}$$

This is identical to (8.18) for $n = 2$, apart for a factor 2. Thus, even if we only used a single point to approximate the integrand in each interval, the estimate of the error is of the same order as the one obtained when we use two points. Indeed, the midpoint method derives from the integrand approximation with a Lagrange polynomial of the first degree passing through two coinciding points lying in the center of the interval.

8.2.3 *The trapezoid rule*

Using a Lagrange polynomial $L_1(x)$ of the first degree passing through the points $(c_i, f(c_i))$ e $(c_{i+1}, f(c_{i+1})$ we obtain the trapezoid or Bézout[3] rule (we leave the determination of $L_1(x)$ as an exercise):

$$I_i = \int_{c_i}^{c_{i+1}} f(x)\, dx \simeq I_i^{(2)} = \int_{c_i}^{c_{i+1}} L_1(x) dx = \frac{f(c_{i+1}) + f(c_i)}{2} (c_{i+1} - c_i) \ ,$$

Its name is due to the fact that from a geometric point of view the integral consists, in fact, to calculating the area of a trapezoid whose bases are equal to $f(a)$ and $f(b)$ with height $(c_{i+1} - c_i)$, as shown in the rightmost plot of Figure 8.1. The error we make when approximating with the trapezoid rule, computed with (8.18), is

$$\delta^{(2)} \leq \frac{1}{12} \left| \sup_{\xi \in [a,b]} f"(\xi) \right| h^2 (b-a) = \frac{1}{12} \left| \sup_{\xi \in [a,b]} f"(\xi) \right| \frac{(b-a)^3}{M^2} \ , \qquad (8.23)$$

i.e., (8.18) with $D_2 = 2/3$. Even if the Lagrange polynomial of degree 1 describes the integrand better than the polynomial of a smaller degree, this does not imply the trapezoid rule is more precise than the rectangle rule. Indeed, the midpoint method, which is a special case of the latter, is a clear case of this. Even if the behavior of δ with n is different, the possible symmetry properties of the interpolating polynomial and the size of the maximum of the n–th derivative of f in the interval $[a, b]$ may produce results which at first sight seem unexpected. To understand this better, let us observe Figure 8.1. In the integration interval the function is shaped such that it overestimates the left subinterval and underestimates the right subinterval. The final result could be that on average the integral of $f(x)$ evaluated in this way is more or less correct. Instead, in case of the trapezoid rule, the integral in Figure 8.1 is underestimated. It must be said that this is not a general rule and which technique is more adapted depends on the type of function. This occurs when the integrand is almost linear, since in that case we have that

$$f\left(\frac{a+b}{2}\right) \simeq \frac{1}{2}(f(a) + f(b)) \, .$$

Thus, in this case both methods are essentially equivalent.

[3] Étienne Bézout (1730-1783) was a French mathematician.

If we know how the error behaves with h, we can adopt a relatively simple technique to estimate the true value of I. By writing

$$I = \sum_{i=0}^{M-1} I_i^{(n)} + R(h)\,, \tag{8.24}$$

the error $R(h)$ is given by the relations (8.20), (8.22) or (8.23), depending on the used method. In all cases, we have that $R(h) = Ah^n$ ($n = 1$ for the rectangle rule and $n = 2$ in the other two cases) and the following relation is valid

$$\lim_{h\to 0} R(h) = 0\,.$$

In this limit, we can extrapolate the true value of the integral. By evaluating $\sum_i I_i$ for different sizes h of the interval, we can plot the results as a function of h^n and perform a linear regression on the data obtained in this way. Relation (8.24) tells us that the intercept of the straight line interpolating the data represents the best estimator of the value I.

If the integrand is sufficiently regular, the method allows us to limit M to few points, thus limiting the computational cost. So, it is not always true that the size h of the interval should be very small. Due to rounding errors, actually, the contrary can be true.

Hands on 5 - Comparing integration methods

Write a program to numerically evaluate the integral of a function you are able to integrate also analytically, with the three different methods described in this section. Allow the user to give the integration interval $[a, b]$ and the minimum $M_{\min}$ and maximum $M_{\max}$ number of parts in which it should be divided. Compute the integral $I(m)$ for m comprised between $M_{\min}$ and $M_{\max}$ and plot the values of $I(m)$ as a function of h or h^2, depending on the cases. Perform a linear regression on the resulting behaviors and compare the intercept with the true value of the integral. Try with the functions $\sin(x)$ and $\sin(1/x)$ in the interval $[0, \pi]$ with $1 < m < 100$. The first is approximately equal to 0.4597, the second to 1.5759.

When we write a function for numerical integration, we always need to pay attention to possible rounding problems we already discussed several times. Indeed, if the number M of points dividing the interval is large, it is appropriate to adopt accurate summation algorithms, like the Kahan algorithm (Section 4.5). A sloppy encoding could cause problems when M is small. Let us consider Listing 8.3, in which the arguments of the `midpoint` function are the endpoints of the integration interval of the function `f`, the number of points in which it is divided and the pointer to the integrand. The integration step `h` is evaluated and a summation cycle is performed until the variable `x` exceeds the value of the right end `b`. For example, if we apply this algorithm to evaluate $\int_0^1 \sin x \, dx$ (this is the integral of a very regular function for which we expect few points should be enough) we find $I_i(M)$ to behave as a function of the number M of points as is given in Figure 8.2. The cause of this strange behavior is once more due to approximation problems. Indeed, certain values of M are completely inadequate, because the corresponding values of h are not exactly representable in the computer memory.

```
1 double midpoint(double a, double b, int m,
2                 double (*f)(double)) {
3   double I = 0., x = a;
4   double h = (b - a) / (double) m;
5   while (x < b) {
6     I += (*f)(x + 0.5 * h);
7     x += h;
8   }
9   return I * h;
10 }
```

Listing 8.3 A bad encoding of the midpoint algorithm.

For example, the value $M = 10$, leads to a value $h = 0.1$, which unfortunately cannot be represented with a finite number of bits in the computer memory[4]. Even though `h` is defined as a `double`, its value is approximated and results are slightly less than the true value. This small difference is sufficient to satisfy the condition on line 5 of the Listing 8.3 at each step, also at the one (the eleventh one) in which we expect it to become false. In this way, the integration interval increases by about 10 percent. Again, a tiny error (of the order of 2^{-64}) causes a disastrous result.

To avoid this type of errors it is better to control the number of steps

[4]The only numbers which can be represented in an exact way are those which can be written as a finite sum of powers of 2.

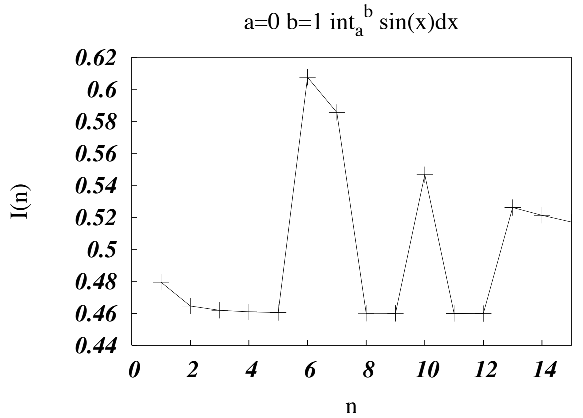

Fig. 8.2 Behavior of the integral $\int_0^1 \sin x dx$ (whose true value is about 0.4597, represented by the dotted line) as a function of M. The estimate is obtained with the midpoint method, dividing the interval $[0, 1]$ in M parts.

rather than the value of x, as is done in the algorithm of Listing 8.4.

```
double midpoint(double a, double b, int m, double (*f)(double)) {
  double I = 0., x, h = (b - a) / (double) m;
  int i;
  for (i = 0; i < m; i++) {
    x = a + h * i + 0.5 * h;
    I += (*f)(x);
  }
  return I * h;
}
```

Listing 8.4 A good encoding of the midpoint algorithm.

8.2.4 *Other integration methods*

To enhance the precision with which the integrand is described inside the integration interval, we can interpolate it with a parabola passing through the integration limits and the midpoint of the interval. Performing this exercise, it is easily proven that

$$I_i = \int_{c_i}^{c_{i+1}} f(x)\, dx \simeq I_i^{(3)} = \frac{c_{i+1} - c_i}{6} \left[f(c_i) + f(c_{i+1}) + 4f\left(\frac{c_{i+1} + c_i}{2}\right)\right] , \tag{8.25}$$

known as the Cavalieri–Simpson formula[5]. Using the formula (8.25) the value of $\sum_i I_i$ converges more rapidly to I when increasing M. Indeed, we have that

$$\delta^{(3)} \leq (b-a)A_3h^4 = A_3\frac{(b-a)^5}{M^4}\,,$$

where A_3 contains all factors not depending on the number of steps. Note that also in this case, the formula seems to converge faster compared to when we use the error estimate of the degree–2 Lagrange polynomial. Again, this is due to the symmetry properties of the polynomial. Indeed, we obtain the same integral with a Lagrange polynomial of four points, two of which coincide with the midpoint of the integration interval.

The integration methods we analyzed so far, unfortunately depend rather strongly on the choice of points in which we divide the integration interval. Indeed, a wrong choice of the integration points can lead to disastrous results (think of a strongly oscillating periodic function, for which we choose the integration points which are separated exactly by a period). The other way around, a good choice of these points leads to an improvement of the precision without increasing the order of the interpolating polynomial (Simpson's method and the midpoint method). By optimizing the choice of points dividing the integration interval we determine an entire class of quadrature formula known as the *Gaussian formulas*. The Gaussian quadrature formulas all have the following form

$$I(f) \equiv \int_a^b f(x)\,dx \simeq S_n(f) \equiv \frac{b-a}{2}\sum_{i=1}^{n} w_i\,f(x_i)\,. \tag{8.26}$$

The points x_i are called *fundamental points*. The various quadrature formulas differ by the number and position of points dividing the interval $[a,b]$. To determine the values w_i and x_i we require the quadrature formula (8.26) to be exact for the polynomial P_m of degree m with m as high as possible. This means we require

$$S_n(P_m) \equiv S_n\left(\sum_{k=0}^{m} a_k x^k\right) = I(P_m)\,.$$

[5]Bonaventura Cavalieri (1598-1647) was a disciple of Galilei. He first calculated the quadrature formula of a parabola. The British mathematician Thomas Simpson (1710-1761) applied this result to the evaluation of an integral of any possible continuous function.

In order for the quadrature formula (8.26) to be exact for a polynomial of degree m it is necessary and sufficient that for each x^k with $k = 0, \dots, m$:

$$R_n(x^k) \equiv \int_a^b x^k \, dx - \frac{b-a}{2} \sum_{i=1}^{n} w_i x_i^k = 0 \,. \tag{8.27}$$

This relation must be true for each k and represents a system of $m+1$ equations in $2n$ unknowns (n values of w_i and as many x_i). The system can be solved for $m \leq 2n-1$. Therefore, we can find exact quadrature formulas at n points for polynomials of maximum degree $m = 2n-1$. The midpoint formula is a special case of the Gaussian quadrature formula. Even though we assume the function to be constant within the interval, it is also exact for degree–1 polynomials. Indeed, for $n = 1$ we have $m = 2n - 1 = 1$. It is easily verified that the quadrature formula (8.26) with $n = 1$ is exact for degree–1 polynomials:

$$\int_a^b P_1(x)\, dx = \int_a^b (Ax+B)\, dx = \left(A\frac{x^2}{2} + Bx \right)\Bigg|_a^b = A\frac{b^2}{2} + Bb - A\frac{a^2}{2} - Ba =$$
$$= \frac{A}{2}\left(b^2 - a^2\right) + B\,(b-a) = (b-a)\left(A\frac{b+a}{2} + B \right) = (b-a)P_1\left(\frac{b+a}{2} \right) ,$$

This is exactly the Gaussian quadrature formula with $w_0 = 2$. More generally, the system (8.27) can be solved for $m = 2n-1$. However, its solutions are not guaranteed to be such that $x_i \in [a,b]$ $\forall i = 1,\dots,n$. We write the polynomial of maximum degree $m = 2n-1$ as $P_m = (x-x_1)\dots(x-x_n)P_{n-1}$. If the Gaussian quadrature formula has to be exact for this polynomial, the following relation must be true

$$\int_a^b (x-x_1)\dots(x-x_n)P_{n-1}\, dx = \frac{b-a}{2} \sum_{i=1}^{n} w_i P_{2n-1}(x_i) = 0 \,. \tag{8.28}$$

This equality derives from the fact that, by construction, $P(x_i) \equiv 0$ $\forall i = 1,\dots,n$. Due to equation (8.28) the fundamental points coincide with the zeros of the polynomial $\Psi_n(x) = (x-x_1)\dots(x-x_n)$. Multiplying the expression (8.27) of the remainder by $\Psi_n(x)$ we have

$$\int_a^b \Psi_n(x) x^k \, dx = \frac{b-a}{2} \sum_{i=1}^{n} w_i \Psi_n(x_i) x_i^k \,. \tag{8.29}$$

It can be shown [Rossetti (1978)] that it is always possible to find a polynomial of degree n which is *orthogonal* to all other polynomials of lower degree with all zeros lying inside the interval $[a, b]$. Two polynomials $\Psi_n(x)$ and $\Psi_m(x)$ are said to be orthogonal in $[a, b]$ if

$$\int_a^b \Psi_n(x)\Psi_m(x)\, dx \propto \delta_{nm}\,.$$

If we can find a base of orthogonal polynomials in $[a, b]$ whose zeros all lie within this interval, we can use the zeros of the degree–n polynomials as fundamental points of the Gaussian quadrature formula of order n. In this way, the system (8.27) is automatically satisfied. The techniques used to determine these polynomials are beyond the scope of this book. The interested reader can find their derivation in [Rossetti (1978)]. A good base of orthogonal polynomials consists of the Legendre polynomials. We can generate a Legendre polynomial $P_j(x)$ of degree j with the relation

$$j\, P_j = (2j-1)\, xP_{j-1} - (j-1)\, P_{j-2}\,, \tag{8.30}$$

with $P_0(x) = 1$ and $P_1(x) = x$. All its zeros are contained in the interval $[-1, 1]$. For this reason the integral is rewritten by substituting the variable

$$y = -\frac{2}{a-b}\, x + \frac{a+b}{a-b}\,,$$

and we obtain

$$\int_a^b f(x)\, dx = \frac{b-a}{2} \int_{-1}^1 f(y)\, dy\,.$$

In this case, always indicating the roots of the polynomial with x_i, it can be shown that

$$w_i = \frac{2}{(1-x_i^2)\left(P'_{n+1}(x_i)\right)^2}\,,$$

where $P'_{n+1}(x_i)$ is the first derivative of the Legendre polynomial of degree $n+1$ evaluated in the point x_i.

Hands on 6 - Gauss-Legendre integration

Using the relation (8.30), write a function returning the generic Legendre polynomial of degree j for a given value of x. Use the bisection method to find its j roots in the interval $[-1, 1]$. To this purpose, keep in mind that the zeros of the Legendre polynomials are symmetric with respect to the origin. Thus, it is enough to find $j/2$ roots in the interval $[0, 1]$ to know all of them. Moreover, the zeros of the polynomial $P_{j+1}(x)$ are distributed such that each one of them lies in an interval given by dividing the segment $[a, b]$ by the roots of $P_j(x)$. Use this property to determine the endpoints delimiting the zeros.

Write a function filling an array with the zeros of the Legendre polynomial of degree $n + 1$ found in the interval $[-1, 1]$ and another array containing the corresponding values of its derivative in those points. The derivative can be approximated with the finite difference ratio

$$P'_{n+1}(x_j) \simeq \frac{P_{n+1}(x_j + \epsilon) - P_{n+1}(x_j)}{\epsilon},$$

where ϵ is the tolerated error when applying Newton's method to find the roots x_j. However, in this case, the equation (8.30) supplies us with a way to compute the exact derivative, namely as

$$jP'_j = (2j - 1)\, P_{j-1} + (2j - 1)\, xP'_{j-1} - (j - 1)\, P'_{j-2}\,.$$

Another function could fill an array containing the coefficients w_i, if the polynomial's zeros and its derivatives are given in input.

At this point, you can compute the integral of any function with the Gauss–Legendre method. Use the program to determine the values of x_i for $n = 2$. If the code is well written, you should find the values $\pm\sqrt{3}/3$. Compare this to your results. Compare the value of the integral of whatever function computed with the 2-point Gauss-Legendre method and the trapezoid rule (in particular, try to integrate a second degree polynomial). Note how the trapezoid method takes the same number of points, but the choice of the abscissa of these points is not optimal.