Because we have taken the expansion symmetrically around x_i all the terms with odd derivatives will drop out because their integral is 0 and we are left with:

$$\int_{x_{i-1}}^{x_{i+1}} f(x)\ \mathrm{d}x = f(x_i) * 2h + f''(x_i) * \frac{2h^3}{3*2!} + \mathcal{O}(h^5 f^{(4)}(x_i)) \tag{6.10}$$

We end up with a result which is of order $h^5 f^{(4)}$. However, we now have to deal with the second derivative. For this we use equation (5.11) from the previous chapter, which we substitute into equation (6.10) to get:

$$\begin{aligned} \int_{x_{i-1}}^{x_{i+1}} f(x)\ \mathrm{d}x &= 2hf(x_i) + \frac{h}{3}(f(x_{i-1}) - 2f(x_i) + f(x_{i+1})) + \mathcal{O}(h^5 f^{(4)}(x_i)) \\ &= h\left(\frac{1}{3}f(x_{i-1}) + \frac{4}{3}f(x_i) + \frac{1}{3}f(x_{i+1})\right) + \mathcal{O}(h^5 f^{(4)})(x_i)) \end{aligned} \tag{6.11}$$

As the last step we extend this for the whole interval $[a, b]$ to end up with:

$$\int_a^b f(x)\ \mathrm{d}x = \frac{h}{3}(f(a) + 4f(a+h) + 2f(a+2h) + 4f(a+3h) + \cdots + f(b)) \tag{6.12}$$

Remember, we are using *three* points for our integration. This requires that the number of intervals is even and therefore the number of points is odd.

6.3 More advanced integration

Gaussian integration with Legendre polynomials

We will now turn our attention to a more sophisticated technique of integration. All the previous methods can be expressed with the following general approximation:

$$\int_a^b f(x)\ \mathrm{d}x = \sum_{i=1}^{N} f(x_i) w_i \tag{6.13}$$

where w_i is the corresponding weight for $f(x_i)$. In the case of the trapezoidal method the weights are $(h/2, h/2)$, and in the case of the Simpson method the weights are $(h/3, 4h/3, h/3)$. In addition, the points x_i are separated equidistantly. These integrations are also known as quadrature, and we can consider them as approximations of the integrands by polynomials in each slice. The next form, Gauss–Legendre integration, will approximate the integrand with a polynomial over the whole interval. The fundamental idea behind this method lies in the fact that we can express a function $f(x)$ in an interval $[a, b]$ in terms of a complete set of polynomials P_l,

$$f(x) = \sum_{l=0}^{n} \alpha_l P_l \tag{6.14}$$

As you will see below, it is convenient to choose orthogonal polynomials, and the first such set we will use are the Legendre[3] polynomials, which have the following property:

$$\int_{-1}^{+1} P_n(x) P_m(x) = \frac{2}{2m+1} \delta_{n,m} \tag{6.15}$$

Because these polynomials are only defined in $[-1, 1]$, we have to change our integration limits from $[a, b] \rightarrow [-1, 1]$ by the following substitution:

$$x \rightarrow \frac{b-a}{2} x + \frac{b+a}{2} \tag{6.16}$$

leading to

$$\int_a^b f(x)\ \mathrm{d}x \rightarrow \frac{b-a}{2} \int_{-1}^{+1} f\left(\frac{b-a}{2} x + \frac{b+a}{2}\right)\ \mathrm{d}x \tag{6.17}$$

For some functions, other polynomials will be more convenient, and you will have to remap your integral limits to those for which the polynomials are defined. Because this remapping is trivial, for the following discussion, we will assume that we are only interested in the integral in $[-1, 1]$.

As the starting point for our discussion we will assume that the function $f(x)$ can be approximated by a polynomial of order $2n-1$, $f(x) \approx p_{2n-1}(x)$. If this is a good representation we can express our integral with:

$$\int_{-1}^{+1} f(x)\ \mathrm{d}x = \sum_{i=1}^{n} w_i f(x_i) \tag{6.18}$$

In other words, knowing the n abscissas x_i and the corresponding weight values w_i we can compute the integral. This means that we have to find out how to determine these quantities. In the first step we will decompose p_{2n-1} into two terms

$$p_{2n-1}(x) = p_{n-1}(x) P_n(x) + r_{n-1} \tag{6.19}$$

[3] Adrien-Marie Legendre, 1752–1833, French mathematician.

where P_n is a Legendre polynomial of order n, while p_{n-1} and r_{n-1} are polynomials of order $(n-1)$. Expressing p_{n-1} by Legendre polynomials as well, we get

$$\int_{-1}^{+1} p_{2n-1}(x)\ \mathrm{d}x = \sum_{k=0}^{n-1} \alpha_k \int_{-1}^{+1} P_k(x) P_n(x)\ \mathrm{d}x + \int_{-1}^{+1} r_{n-1}(x)\ \mathrm{d}x \tag{6.20}$$

Because of the orthogonality, the first term vanishes and we are left with:

$$\int_{-1}^{+1} p_{2n-1}(x)\ \mathrm{d}x = \int_{-1}^{+1} r_{n-1}(x)\ \mathrm{d}x \tag{6.21}$$

Furthermore, we know that P_n has n zeros in $[-1, +1]$, which we will label $x_1, x_2, \ldots, x_n$. For these points we have the relation:

$$p_{2n-1}(x_i) = r_{2n-1}(x_i) \tag{6.22}$$

Expressing $r_{n-1}(x)$ with Legendre polynomials

$$r_{n-1}(x) = \sum_{k=0}^{n-1} w_k P_k(x) \tag{6.23}$$

and using equation (6.22) we finally get:

$$p_{2n-1}(x_i) = \sum_{k=0}^{n-1} w_k P_k(x_i) \tag{6.24}$$

The $P_k(x_i)$ are the values of the Legendre polynomials of order k, up to $k = n-1$ evaluated at the roots x_i of the Legendre polynomial $P_n(x)$.
If we write this out for $k = 2$ we get:

$$\begin{aligned}
p_{2n-1}(x_1) &= w_0 P_0(x_1) + w_1 P_1(x_1) + w_2 P_2(x_1) \\
p_{2n-1}(x_2) &= w_0 P_0(x_2) + w_1 P_1(x_2) + w_2 P_2(x_2) \\
p_{2n-1}(x_3) &= w_0 P_0(x_3) + w_1 P_1(x_3) + w_2 P_2(x_3)
\end{aligned}$$

which we can write conveniently in matrix form:

$$p_{2n_1}(x_1, \ldots, x_n) = \begin{pmatrix} P_0(x_1) & P_1(x_1) & \ldots & P_k(x_1) \\ \multicolumn{4}{c}{\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots} \\ P_0(x_n) & P_1(x_n) & \cdots & P_k(x_n) \end{pmatrix} \begin{pmatrix} w_0 \\ w_1 \\ \\ \\ w_k \end{pmatrix} \tag{6.25}$$

In order to solve for the unknown w_k we have to invert the matrix $\mathbf{P}$:

$$w_k = \sum_{i=1}^{n} p_{2n-1}(x_i) \{\mathbf{P}^{-1}\}_{ik} \tag{6.26}$$

Finally, after all this mathematical hoopla we get back to our integral:

$$\int_{-1}^{+1} f(x)\ \mathrm{d}x = \int_{-1}^{+1} p_{2n-1}(x)\ \mathrm{d}x = \sum_{k=0}^{n-1} w_k \int_{-1}^{+1} P_k(x)\ \mathrm{d}x \tag{6.27}$$

Using the fact that $P_{k=0}(x) = 1$, we can multiply this equation with $P_0(x)$ and use the orthogonality condition to get

$$\int_{-1}^{+1} p_{2n-1}(x)\ \mathrm{d}x = 2w_0 = 2\sum_{i=1}^{n} p_{2n-1}(x_i)\{\mathbf{P}^{-1}\}_{i0} \tag{6.28}$$

since

$$\int_{-1}^{+1} P_k(x)P_0(x)\ \mathrm{d}x = \frac{2}{2k+1}\delta_{k,0} \tag{6.29}$$

from the properties of the Legendre polynomials. Up to now we have assumed that $f(x)$ is exactly represented by a polynomial, while in most cases this is an approximation:

$$p_{2n-1}(x_i) \approx f(x_i) \tag{6.30}$$

Using equation (6.30) we can express our integral as

$$\int_{-1}^{+1} f(x)\ \mathrm{d}x = \sum_{i=1}^{n} f(x_i)w_i \tag{6.31}$$

with

$$w_i = 2\{\mathbf{P}^{-1}\}_{i0} \tag{6.32}$$

The w_i is the weight of $f(x_i)$ at the zeros of $P_n(x)$ and can be calculated. However, these values are also tabulated, for example by Abramowitz and Stegun in the *Handbook of Mathematical Functions* [6]. The following table lists the values for $n = 4$ and $n = 5$.

Order	Abscissa x_i	Weight w_i
$n = 4$	±0.339981043584856	0.652145154862546
	±0.861136311594053	0.347854845137454
$n = 5$	±0.000000000000000	0.568888888888889
	±0.538469310105683	0.478628670499366
	±0.906179845938664	0.236926885056189

Gaussian integration with Laguerre polynomials

The drawback of the Gauss–Legendre integration is that the limits have to be finite, because the Legendre polynomials are only defined on $[-1, 1]$. However, many times you will encounter integrals of the form:

$$\int_0^\infty f(x)\ \mathrm{d}x \tag{6.33}$$

or

$$\int_{-\infty}^\infty f(x)\ \mathrm{d}x \tag{6.34}$$

One type of integral commonly encountered in physics is of the type:

$$\int_0^\infty \mathrm{e}^{-x} f(x)\ \mathrm{d}x \tag{6.35}$$

This integral can be calculated using Gauss–Laguerre quadrature, where we are using Laguerre polynomials, which are orthogonal polynomials in the region $[0, \infty]$.

$$\int_0^\infty \mathrm{e}^{-x} f(x)\ \mathrm{d}x = \sum_{k=1}^{N} f(x_k) W_k \tag{6.36}$$

where the x_k are the zeros of the Laguerre polynomials and the W_k are the corresponding weights and are tabulated in [6]. Another way to look at the integration in $[0, \infty]$ is

$$\begin{aligned} \int_0^\infty f(x)\ \mathrm{d}x &= \int_0^\infty \mathrm{e}^{x}\mathrm{e}^{-x} f(x)\ \mathrm{d}x \\ &= \sum_{k=1}^{N} w(x_k)\ \mathrm{e}^{x_k}\ f(x_k) \end{aligned} \tag{6.37}$$

which is also tabulated in Abramowitz and Stegun [6]. You can also find these values at:

http://www.efunda.com/math/num_integration/num_int_gauss.cfm.

Many integrals involving Gaussian distributions are solvable by using Hermitian polynomials $H(x)$, which are defined in $[-\infty, \infty]$

$$\int_{-\infty}^\infty f(x)\ \mathrm{d}x \approx \sum_{k=1}^{N} w_k f(x_k) \tag{6.38}$$

and integrals of the form

$$\int_{-1}^{1} \frac{f(x)\ \mathrm{d}x}{\sqrt{1-x^2}} \tag{6.39}$$

can be solved with Chebyshev polynomials:

$$\int_{-1}^{1} \frac{f(x)\ \mathrm{d}x}{\sqrt{1-x^2}} \approx \sum_{k=1}^{N} w_k f(x_k) \tag{6.40}$$

where in both cases the x_k are the roots of the respective polynomials.

6.4 Exercises

1. Using your sin program, write a new program which integrates

$$f(x) = \int_0^{\pi} \sin(x)\ \mathrm{d}x$$

   with N intervals, where $N = 4,\ 8,\ 16,\ 256$ and 1024 and compare the result for the trapezoid and Simpson methods.
2. Write a general use function or class in which you can give the function and integration limits.
3. Use your created function to solve the problem of a projectile with air resistance to determine the horizontal and vertical distances as well as the corresponding velocities as a function of time. This is a problem which you have to outline carefully before you attack it.
4. Use Laguerre integration to calculate the Stefan–Boltzmann constant.