Chapter 6

Numerical Integration

6.1 Introduction

Numerical integration is the approximate computation of a definite integral using numerical techniques.

There are a wide range of methods available for numerical integration. A good source for such techniques is [NR77]. Numerical integration is implemented in Mathematica as '`NIntegrate[f(x), {x, xmin, xmax}]`'.

The most straightforward numerical integration technique uses the *Newton–Cotes formulae*, which approximate a function tabulated at a sequence of regularly spaced intervals by polynomials of various degree. If the endpoints are tabulated, then the 2- and 3-point formula are called the trapezoidal rule and Simpson's rule, respectively. The 5-point formula is called Boole's rule. A generalization of the trapezoidal rule is Romberg integration, which can yield accurate results for relatively few function evaluations.

If the integrand is known analytically, rather than being tabulated at equally spaced intervals, the best numerical integration method is *Gaussian quadrature*. By cleverly choosing the abscissas at which to evaluate the function, Gaussian quadrature produces the most accurate approximations possible for a given number of function evaluations. However, given the speed of modern computers, the additional complication of Gaussian quadrature often makes it less convenient than simply brute-force calculating twice as many points on a regular grid (which also permits the already computed values of the function to be re-used).

Recall that the definite integral $\int_a^b f(x)\,dx$ is the area under the curve $y = f(x)$ between the limits $x = a$ and $x = b$:

$$\int_a^b f(x)\,dx = \lim_{n\to\infty} \sum_{i=1}^{n} f(\alpha_i)\,(x_i - x_{i-1})\,, \tag{6.1}$$

where $x_{i-1} \le \alpha_i \le x_i$ and $a = x_0 < x_1 < x_2 < x_3 < \ldots < x_n = b$.

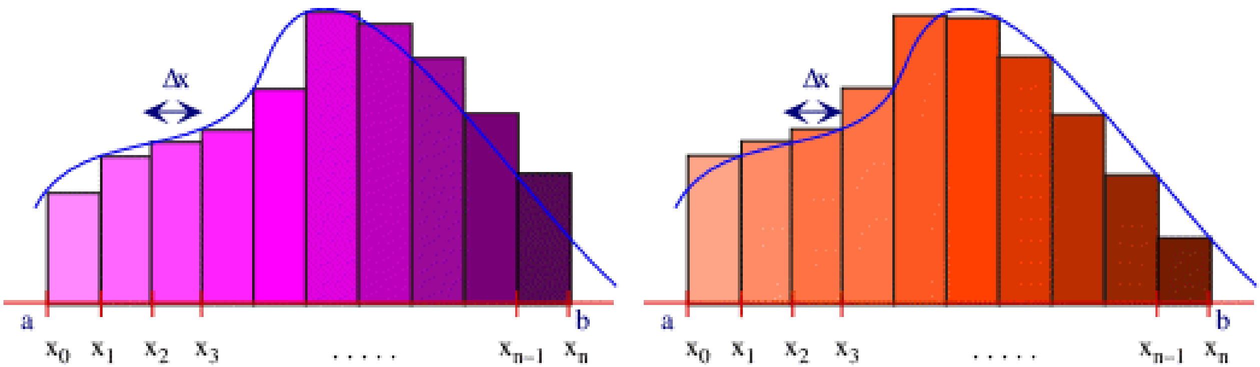

Figure 6.1: Left: Left Riemann sum; the left side of each rectangle matches the height of the graph. *Right:* Right Riemann sum; the right side of each rectangle matches the height of the graph.

6.2 Equidistant formulae

Equidistant integration formulae are formulae that evaluate the integrand at points that have a fixed distance h from their nearest neighbours. In other words, if we integrate from a to b, the *nodes* where we evaluate the function are

$$x_i = a + ih \ , \qquad i = 0, \ldots, n \ , \tag{6.2}$$

where $h = (b-a)/n$, and n is the number of intervals (i.e., the number of nodes minus 1).

6.2.1 Left and right Riemann sums (rectangular rule)

Let us divide the interval into n subintervals of length $h = (b-a)/n$, and in each subinterval choose $\alpha_i = x_{i-1}$ (left Riemann sum), or $\alpha_i = x_i$ (right Riemann sum) as shown in Figs. 6.1. For the left Riemann sum, we get

$$\int_a^b f(x)\,dx \approx h(y_0 + y_1 + y_2 + \ldots + y_{n-1}) \ , \tag{6.3}$$

where $y_0 = f(x_0)$, $y_1 = f(x_1)$ etc.

For the right Riemann sum, we get

$$\int_a^b f(x)\,dx \approx h(y_1 + y_2 + y_3 + \ldots + y_n) \ . \tag{6.4}$$

6.2.2 The trapezoidal rule

The *trapezoidal rule* approximates the function on each interval by a linear function. It thus gives the exact result for constant or linear functions, as can be seen from the error

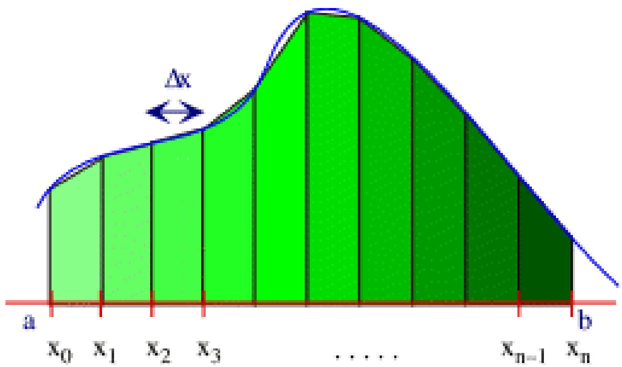

Figure 6.2: The trapezoidal method.

term below.[1]

$$\begin{aligned}\int_{x_1}^{x_n} f(x)\,dx &= \sum_{k=1}^{n-1}\int_{x_k}^{x_{k+1}} f(x)dx \\ &= \underbrace{\sum_{k=1}^{n-1}\frac{h}{2}[f(x_k)+f(x_{k+1})]}_{=h\,\frac{f_1+2f_2+\ldots+2f_{n-1}+f_n}{2}} + O\left(h^3 f''(\xi)\right)\,,\end{aligned} \tag{6.5}$$

where $h = x_{k+1} - x_k$, and $x_1 < \xi < x_n$.

6.2.3 Simpson's rule

Simpson's rule approximates the function on each interval by a parabolic function. It gives the exact result even for arbitrary polynomials of third order.

$$\begin{aligned}\int_{x_1}^{x_n} f(x)\,dx &= \sum_{k=1}^{(n-1)/2}\int_{x_{2k-1}}^{x_{2k+1}} f(x)\,dx \\ &= \underbrace{\sum_{k=1}^{(n-1)/2}\frac{h}{3}[f(x_{2k-1})+4f(x_{2k})+f(x_{2k+1})]}_{=h\,\frac{f_1+4f_2+2f_3+4f_4+\ldots+2f_{n-2}+4f_{n-1}+f_n}{3}} + O\left(h^5 f^{(4)}(\xi)\right)\end{aligned} \tag{6.6}$$

where $h = x_{2k+1} - x_{2k} = x_{2k} - x_{2k-1}$, and $n \geq 3$ is an odd integer number.

[1] Note that ξ in the error term is unknown, so it is generally not possible to explicitly calculate the error term in Eq. (6.5). However, for a linear function f, the second derivative $f''(\xi)$ is identically zero, and thus the error term vanishes.

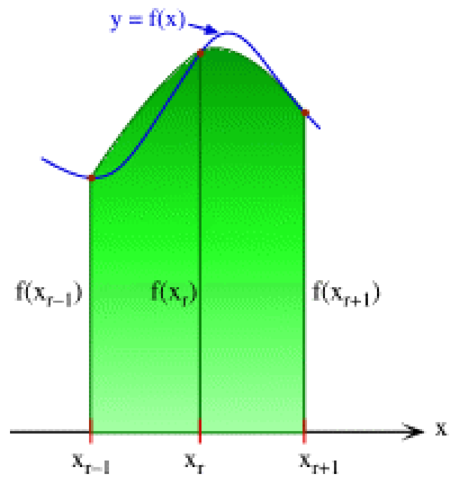

Figure 6.3: Simpson's method.

6.3 Romberg integration

Suppose we approximate the integral $\int_a^b f(x)\,dx$ using the trapezoidal rule with step size h. The value I_1 thus obtained differs from the exact answer I_{exact} by the truncation error, such that[2]

$$I_1 = I_{\text{exact}} + Ch^2 + Dh^4 + Eh^6 + \ldots \tag{6.7}$$

where C, D, E etc. are constants that we treat as unknown. Now suppose that the calculation is repeated with step size $h/2$ to obtain an approximate value I_2

$$I_2 = I_{\text{exact}} + C\left(\frac{h}{2}\right)^2 + D\left(\frac{h}{2}\right)^4 + E\left(\frac{h}{2}\right)^6 + \ldots \tag{6.8}$$

and repeated again with step size $(\frac{h}{4})$ to obtain an approximate value I_3, then

$$I_3 = I_{\text{exact}} + C\left(\frac{h}{4}\right)^2 + D\left(\frac{h}{4}\right)^4 + E\left(\frac{h}{4}\right)^6 + \ldots \tag{6.9}$$

In the three equations above we only know I_1, I_2, I_3, and h.

In each of the above equations, the error is second order (i.e., $\propto h^2$). A more accurate value can be found by algebraically eliminating the h^2 error term from Eq. (6.7) and Eq. (6.8); that is 4×(6.8)−(6.7) to yield

$$I_1^* = I_{\text{exact}} - \frac{1}{4}D\,h^4 - \frac{5}{16}E\,h^6 + \ldots \tag{6.10}$$

where $I_1^* = (4I_2 - I_1)/3$ is a more accurate value for the integral since now the error is $\propto h^4$. Carrying out the same operation for Eqs. (6.8) and (6.9) yields

$$I_2^* = I_{\text{exact}} - \frac{1}{64}D\,h^4 - \frac{5}{1024}E\,h^6 + \ldots \tag{6.11}$$

[2]The fact that only even powers of h enter here is related to the fact that the integral over an antisymmetric function vanishes.

where $I_2^* = (4I_3 - I_2)/3$. Furthermore, we can algebraically eliminate the h^4 error term from Eqs. (6.10) and (6.11) to get an even better answer

$$I_1^{**} = I_{\text{exact}} + \frac{1}{64} E h^6 + \frac{21}{1024} F h^8 + \dots , \tag{6.12}$$

where $I_1^{**} = (16I_2^* - I_1^*)/15$.

It is customary to organize the iteration into a *Romberg table*, in which the first column consists of repeated trapezoidal rule calculation with step size h, $h/2$, $h/4$, $h/8$, etc., and subsequent columns contain the algebraic combinations given above.

Table 6.1: Schematic view of Romberg's integration method.

Step	*Trapez. rule*	*1st extrap.*	*2nd extrap.*	*3rd extrap.*	...	*Nth extrap.*
h	$R(1,1) = I_1$					
$h/2$	$R(2,1) = I_2$	$R(2,2) = I_1^*$				
$h/4$	$R(3,1) = I_3$	$R(3,2) = I_2^*$	$R(3,3) = I_1^{**}$			
$h/8$	$R(4,1) = I_4$	$R(4,2) = I_3^*$	$R(4,3) = I_2^{**}$	$R(4,4) = I_1^{***}$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$		
$h/2^{i-1}$	$R(i,1)$	$R(i,2)$	$R(i,3)$	$R(i,4)$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	
$h/2^{N-1}$	$R(N,1)$	$R(N,2)$	$R(N,3)$	$R(N,4)$	...	$R(N,N)$

So let us denote the elements of the Romberg table as $R(n,m)$; they are shown in Table 6.1. The general recursive formulae are

$$R(1,1) = \frac{b-a}{2}\left[f(a) + f(b)\right] \tag{6.13}$$

$$h = \frac{b-a}{2^n} \tag{6.14}$$

$$R(n+1,1) = \frac{1}{2}R(n,1) + h\sum_{k=1}^{2^{n-1}} f[a + (2k-1)h] \tag{6.15}$$

for the trapezoidal rule (try to derive it yourself), and

$$R(n+1,m+1) = R(n+1,m) + \frac{4^m R(n+1,m) - R(n,m)}{4^m - 1} \tag{6.16}$$

for the successive columns.

Note that the power of the Romberg method lies in the fact that it allows us to compute a sequence of approximations to a definite integral using the trapezoidal rule without re-evaluating the integrand at points where it has already been evaluated. This provides an efficient and computationally affordable algorithm.

6.3.1 Example

- Compute 8 rows and columns in the Romberg table for the integral $\int_{1.3}^{2.19} \frac{\sin x}{x}\,dx$ and show that $R(8,8) = 0.49996\,9818$ (the correct value for the integral is $0.49997\,0103$)

- Use the Romberg algorithm to compute the Bessel function $J_0(1) = \frac{1}{\pi}\int_0^{\pi} \cos(\sin\theta)\,d\theta$ and show that $R(8,8) = 0.76519\,7687$.

6.3.2 Algorithm

Use the following algorithm to integrate $y = e^{-x}\sin(8x^{2/3}) + 1$ over the interval $[0,2]$. Show that after roughly 140 sample points the integral converges to the value of 2.016007.

Romberg

```
Romberg[a_, b_, tol_] := Module[
    {a=N[a_0], b=N[b_0]},
    TrapRule[i_] := Module[{k},
    h = h / 2;
    R[[i+1,1]] = (R[[i,1]])/2 + h Sum[f[a+h (2k-1)], {k,1,m}]
    m = 2m;
];
h = b-a;
m = 1;
close = 1;
j = 1;
R = {{0}};
R[[1,1]] = h/2 (f[a]+f[b]);
Print[R[[j]]];
While[And[j <= 11, tol < close], j++;
    R = Append[R, Table[0,{j}]];
    TrapRule[j-1];
    For[k=1, k <= j-1, k++,
        R[[j,k+1]] = R[[j,k]] + (R[[j,k]]-R[[j-1,k]]) / (4^k-1);
    ];
    Print[R[[j]]];
    close = Abs[R[[i,j]]-R[[j-1,j-1]]];
];
Return[R[[j,j]];
];
```

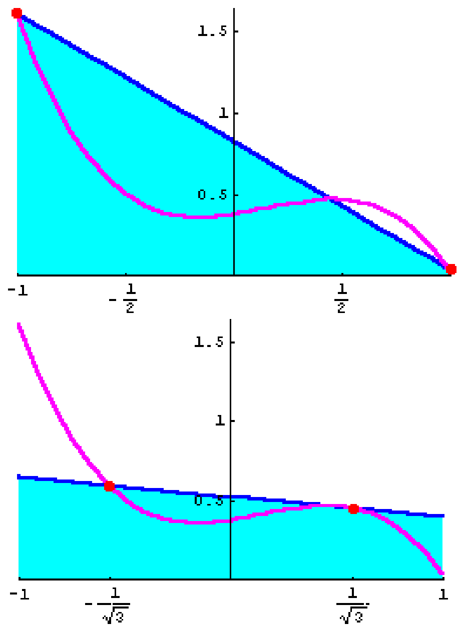

Figure 6.4: Trapezoidal rule (top) vs. Gaussian quadrature (bottom). When the graph of $y = f(x)$ is concave, the error in approximation is the entire region that lies between the curve and the line segment joining the points (e.g. when using the trapezoidal rule). If we are permitted to use the nodes x_1 and x_2 that lie inside the interval [-1,1], the line through the two points $(x_1, f(x_1))$ and $(x_2, f(x_2))$ crosses the curve, and the area under the line more closely approximates the area under the curve.

6.4 Gaussian quadrature

The general quadrature formula approximates an integral by a sum of the form the following form

$$\int_a^b \omega(x)\, f(x)\, dx = \sum_{i=1}^{n} w_i\, f(x_i) + R_n \,, \tag{6.17}$$

where $\omega(x)$ is a weight function whose integral over the interval $[a, b]$ is positive. The n numbers x_i are called *nodes* and the n numbers w_i are called *weights*. The nodes and the weights are chosen such that the right hand side is exact for all polynomials up to a certain order. The error term is R_n.

Gaussian quadrature formulae, which have non-uniformly spaced grid points, are very efficient for known smooth functions. The main idea is to choose not only the weighting coefficients (weight factors) but also the locations (abscissas) where the function $f(x)$ is evaluated (see Figure 6.4 for an illustration). As a result, Gaussian quadrature yields twice as many places of accuracy as that of equal space formulae with the same number of function evaluations.

We shall see that this method has one further significant advantage in many situations. In the evaluation of an integral on the interval a and b, it is not necessary to evaluate f(x) at the endpoints, i.e. at a and b, of the interval. This will prove valuable when evaluating various improper integrals, such as those with infinite limits.

6.4.1 Gaussian quadrature with arbitrary polynomials

We first illustrate the technique for $\omega(x) = 1$. For fixed nodes $\{x_i\}$, the theory of polynomial interpolation states that there is a corresponding *Lagrange interpolation formula*

$$p(x) = \sum_{i=1}^{n} f(x_i)\, l_i(x) \quad \text{where} \quad l_i(x) = \prod_{\substack{j=1,\\ j\neq i}}^{n} \frac{x - x_i}{x_i - x_j} \tag{6.18}$$

(see § 4.2.2). This formula provides a polynomial of degree $\leq n{-}1$ that interpolates f at the nodes, i.e. that satisfies $p(x_i) = f(x_i)$ for $1 \leq i \leq n$.

Now we can simply write

$$\int_a^b f(x)\, dx \simeq \int_a^b p(x)\, dx = \sum_{i=1}^{n} f(x_i) \int_a^b l_i(x)\, dx = \sum_{i=1}^{n} w_i f(x_i) \tag{6.19}$$

where (as you may have guessed by now) the weights are

$$w_i = \int_a^b l_i(x)\, dx\ . \tag{6.20}$$

Example: Determine the quadrature formula when the interval is $[a, b] = [-2, 2]$ and the nodes are $-1, 0, 1$.

Here we have:

$$l_1(x) = \prod_{\substack{j=1,\\ j\neq 1}}^{3} \frac{x - x_i}{x_i - x_j} = \frac{x-0}{-1-0}\,\frac{x-1}{-1-1} = \frac{1}{2}(x^2 - x)\ . \tag{6.21}$$

Similarly, $l_2(x) = -x^2 + 1$ and $l_3(x) = \frac{1}{2}(x^2 + x)$. The weights are then obtained by integrating these functions:

$$w_1 = \int_{-2}^{2} l_1(x)\, dx = 8/3\ , \tag{6.22}$$

and $w_2 = -4/3$, $w_3 = 8/3$. The quadrature formula for any function $f(x)$ for the specified nodes is then

$$\int_{-2}^{2} f(x)\, dx \;\simeq\; \frac{8}{3} f(-1) - \frac{4}{3} f(0) + \frac{8}{3} f(1)\ . \tag{6.23}$$

(Verify that this gives correct values for $f(x) = 1, x$ and x^2.)

6.4.2 Gaussian quadrature with orthogonal polynomials

The fundamental theorem of Gaussian quadrature states that the optimal abscissas of the N-point Gaussian quadrature formulae are precisely the roots of the orthogonal polynomial for the same interval and weighting function. Gaussian quadrature is optimal because it fits all polynomials up to degree $2N$ exactly.

More specifically:

- With arbitrary nodes (associated with roots of arbitrary polynomials), formula (6.17) will be exact for all polynomials of degree $\leq n-1$.
- With Gaussian nodes (associated with roots of orthogonal polynomials), formula (6.17) will be exact for all polynomials of degree $\leq 2n-1$.

An important case where the Gaussian formulae have a serious advantage occurs in integrating a function that is infinite at one end of the interval or has there some other singularity. The reason for this advantage is that the nodes in Gaussian quadrature are always interior points of the interval. Thus, for example, when computing $\int_0^1 \frac{\sin x}{x}\,dx$, the Fortran statement '`y=sin(x)/x`' can be safely used with a Gaussian formula since the function will not be evaluated at $x = 0$. More difficult integrals such as $\int_0^1 (x^2-1)^{1/3}[\sin(e^x - 1)]^{-1/2}\,dx$ can be computed directly with a Gauss formula in spite of the singularity at 0.

In summary, all Gaussian quadrature rules have the format;

$$\int_a^b \omega(x)\, f(x)\, dx = \sum_{k=1}^{n} w_k f(x_k) + R_n \ , \tag{6.24}$$

where x_k, associated with zeros of orthogonal polynomials, are the integration points. Table 6.2 summarizes the 4 most common types of weight function $\omega(x)$ and orthogonal polynomials $p(x)$ used for Gaussian quadrature.

Table 6.2: Characteristics of the most popular Gaussian quadrature methods.

Interval	$\omega(x)$	*Related Orthogonal Polynomials*
$[-1,1]$	1	Legendre Polynomials $P_n(x)$
$[-1,1]$	$1/\sqrt{1-x^2}$	Chebyshev Polynomials $T_n(x)$
$[0,\infty]$	e^{-x}	Laguerre Polynomials $L_n(x)$
$[-\infty,\infty]$	e^{-x^2}	Hermite Polynomials $H_n(x)$

6.4.3 Gauss–Legendre formula [$\omega(x) = 1$]

The simplest form of Gaussian Integration is based on the use of an optimally chosen polynomial to approximate the integrand $f(x)$ over the interval $[-1,+1]$.

$$\int_a^b f(x)\,dx = \int_{-1}^{1} f\left(\frac{b-a}{2}\,x' + \frac{b+a}{2}\right)\frac{b-a}{2}\,dx' \tag{6.25}$$

$$= \frac{b-a}{2}\int_{-1}^{1} g(x')\,dx' = \frac{b-a}{2}\sum_{k=1}^{n} w_k\, g(x'_k) + R_n \tag{6.26}$$

$$= \frac{b-a}{2}\sum_{k=1}^{n} w_k\, f\left(\frac{b-a}{2}\,x'_k + \frac{b+a}{2}\right) + R_n\ , \tag{6.27}$$

where

$$x' \equiv \frac{x - \frac{b+a}{2}}{\frac{b-a}{2}}\ , \qquad \text{i.e.} \qquad x = \frac{b-a}{2}\,x' + \frac{b+a}{2}\ , \qquad -1 < x' < 1\ , \tag{6.28}$$

x'_k is the k-th zero of $P_n(x')$,

$$w_k \equiv \frac{2}{(1-x_k'^{2})\,[P'_n(x'_k)]^2}\ , \tag{6.29}$$

$$g(x') \equiv f\left(\frac{b-a}{2}\,x' + \frac{b+a}{2}\right), \tag{6.30}$$

and the residual term is

$$R_n = \frac{2^{2n+1}(n!)^4}{(2n+1)\,[(2n)!]^3}\; g^{(2n)}(\xi)\ , \tag{6.31}$$

where $-1 < \xi < 1$, and $g^{(2n)}(\xi)$ denotes the $2n$-th derivative of the function $g(\xi)$.

The Gauss–Legendre integration formula is the most commonly used form of Gaussian quadratures. It is based on the Legendre polynomials of the first kind $P_n(x)$. In Mathematica, these polynomials are called '`LegendreP[n,x]`' and the k-th node can be found by calling '`Root[LegendreP[n,x], k]`'.

Nodes and weights for the 2-, 3-, and 4-point formulae are listed in Table 6.3.

Application

Consider the evaluation of the integral:

$$I = \int_0^{\pi/2} \sin x\, dx\ , \tag{6.32}$$

whose value is 1, as obtained by explicit integration. After transforming the integral to the interval $[-1, 1]$, we apply the 2-point Gaussian method, using the nodes and wights given in Table 6.3.

Table 6.3: Nodes and weights for the 2-, 3-, and 4-point Gauss–Legendre rule.

	x_k	w_k
2-point:	$\pm\sqrt{\frac{1}{3}}$	1
3-point:	0	$\frac{8}{9}$
	$\pm\sqrt{\frac{3}{5}}$	$\frac{5}{9}$
4-point:	±0.33998 10435 84856	0.65214 515486 2546
	±0.86113 63115 94052	0.34785 484513 7454

The calculation is simply:

$$I \approx \frac{\pi}{4}\left\{1.0 \times \sin\left[\left(1-\frac{1}{\sqrt{3}}\right)\frac{\pi}{4}\right] + 1.0 \times \sin\left[\left(1+\frac{1}{\sqrt{3}}\right)\frac{\pi}{4}\right]\right\} \tag{6.33}$$

$$\approx 0.998473\,, \tag{6.34}$$

which is pretty close to the exact value of 1. While this example is quite simple, the values shown in Table 6.4 indicate how accurate the estimate of the integral is for only a few function evaluations. The table includes a column of values obtained from Simpson's rule for the same number of function evaluations. While the results based on 2 points have similar accuracy, the accuracy of the Gauss–Legendre approximation increases drastically with the number of nodes.

Table 6.4: Comparison of Gauss–Legendre integration and Simpson's rule, applied to the integral (6.32).

N	*Gauss–Legendre*	*Simpson*
2	0.9984726134	1.0022798775
4	0.9999999772	1.0001345850
6	1.0000000000	1.0000263122
8	1.0000000000	1.0000082955
10	1.0000000000	1.0000033922

6.4.4 Gauss–Chebyshev formula [$\omega(x) = 1/\sqrt{1-x^2}$]

This method is used for integrating over the interval $[a, b]$ with a weighting function $1/\sqrt{(x-a)(b-x)}$ and is based on the Chebyshev polynomials of the first kind $T_n(x)$.

$$\int_a^b f(x)\,dx \;=\; \int_a^b \frac{\sqrt{(x-a)(b-x)}\,f(x)}{\sqrt{(x-a)(b-x)}}\,dx \tag{6.35}$$

$$= \int_{-1}^{1} \frac{g(x')}{\sqrt{1-x'^2}}\,dx' \;=\; \sum_{k=1}^{n} w_k\,g(x'_k) + R_n \tag{6.36}$$

$$= \frac{b-a}{2}\sum_{k=1}^{n} w_k\,\sqrt{1-x_k'^2}\;f\!\left(\frac{b-a}{2}\,x'_k + \frac{b+a}{2}\right) + R_n\;, \tag{6.37}$$

where

$$x' \equiv \frac{x-\frac{b+a}{2}}{\frac{b-a}{2}}\;, \qquad \text{i.e.} \qquad x = \frac{b-a}{2}\,x' + \frac{b+a}{2}\;, \qquad -1 < x' < 1\;, \tag{6.38}$$

and

$$x'_k \;\equiv\; \cos\frac{(2k-1)\,\pi}{2n}\;, \tag{6.39}$$

$$w_k \;\equiv\; \frac{\pi}{n}\;, \tag{6.40}$$

$$g(x') \;\equiv\; \frac{b-a}{2}\,\sqrt{1-x'^2}\;f\!\left(\frac{b-a}{2}\,x' + \frac{b+a}{2}\right), \tag{6.41}$$

and the residual term is

$$R_n = \frac{\pi}{2^{2n-1}\,(2n)!}\;g^{(2n)}(\xi)\;, \tag{6.42}$$

where $-1 < \xi < 1$, and $g^{(2n)}(\xi)$ denotes the $2n$-th derivative of the function $g(\xi)$.

In Mathematica, the Chebyshev polynomials are called '`ChebyshevT[n,x]`' and the k-th node can be found by calling '`Root[ChebyshevT[n,x], k]`' [which is a very expensive way to evaluate Eq. (6.39)].

For example let us integrate

$$I = \int_{-1}^{1} \sqrt{(1-x^2)}dx\;. \tag{6.43}$$

First we need to rewrite I as

$$I = \int_{-1}^{1} \frac{1-x^2}{\sqrt{1-x^2}}dx\;. \tag{6.44}$$

We leave it to the reader to show that $I = 1.570796327$ using only 3 Chebyshev nodes.

6.4.5 Gauss–Hermite formula [$\omega(x) = e^{-x^2}$]

This method is applicable for infinite integrals over the interval $[-\infty, \infty]$ and is based on the Hermite polynomials $H_n(x)$.

$$\int_{-\infty}^{\infty} f(x)\,dx = \int_{-\infty}^{\infty} e^{-x^2}\left[e^{x^2} f(x)\right] dx \tag{6.45}$$

$$= \sum_{k=1}^{n} w_k\, e^{x_k^2} f(x_k) + R_n\ , \tag{6.46}$$

where x_k is the k-th zero of the Hermite polynomial $H_n(x)$,

$$w_k \equiv \frac{2^{n-1}\, n!\, \sqrt{\pi}}{n^2\,[H_{n-1}(x_k)]^2}\ , \tag{6.47}$$

$$R_n \equiv \frac{n!\,\sqrt{\pi}}{2^n\,(2n)!}\, f^{(2n)}(\xi)\ , \tag{6.48}$$

where $-\infty < \xi < \infty$, and $f^{(2n)}(\xi)$ denotes the $2n$-th derivative of the function $f(\xi)$.

In Mathematica, the corresponding polynomials are called '`HermiteH[n,x]`' and the k-th node can be found by calling '`Root[HermiteH[n,x], k]`'.

The coefficients for 2- and 5-point Gauss–Hermite integration are listed in Table 6.5.

Table 6.5: Nodes and weights for 2- and 5-point Gauss–Hermite integration.

	x_k	w_k
2-point:	$\pm\sqrt{\frac{1}{2}}$	$\frac{\sqrt{\pi}}{2}$
5-point:	0.00000 000	0.94530 872
	±0.95857 246	0.39361 932
	±2.02018 287	0.01995 324

Application

Calculate the following integrals

$$\int_{-\infty}^{\infty} e^{-x^2} \cos x\, dx; \quad \int_{-\infty}^{\infty} e^{-x^2+x}\, dx \tag{6.49}$$

using 2- and 5-point order Gauss–Hermite quadrature rules.

To within single precision, the 5-point result can be considered as the exact value for the integrals. How accurate is the 2-point result?

6.4.6 Gauss–Laguerre formula [$\omega(x) = e^{-x}$]

This method is used for integration over the semi-infinite interval $[0, \infty]$ and is based on the Laguerre polynomials $L_n(x)$.

$$\int_0^\infty f(x)\,dx = \int_0^\infty e^{-x}\left[e^x f(x)\right]\,dx \tag{6.50}$$

$$= \sum_{k=1}^{n} w_k\, e^{x_k}\, f(x_k) + R_n\,, \tag{6.51}$$

where x_k is the k-th zero of the Laguerre polynomial $L_n(x)$,

$$w_k \equiv \frac{x_k}{(n+1)^2\,[L_{n+1}(x_k)]^2}\,, \tag{6.52}$$

$$R_n \equiv \frac{(n!)^2}{(2n)!}\, f^{(2n)}(\xi)\,, \tag{6.53}$$

where $0 < \xi < \infty$, and $f^{(2n)}(\xi)$ denotes the $2n$-th derivative of the function $f(\xi)$.

In Mathematica, the corresponding polynomials are called '`LaguerreL[n,x]`' and the k-th node can be found by calling '`Root[LaguerreL[n,x], k]`'

Application

Consider the gamma function defined by

$$\Gamma(\alpha) = \int_0^\infty e^{-x} x^{\alpha-1}\,dx\,. \tag{6.54}$$

Use the formula above to evaluate $\Gamma(1.0), \Gamma(1.4), \Gamma(2.0)$. Compare your results to what you get from Mathematica's function '`Gamma[z]`'.

6.5 Integrals with discontinuities

For later sections

6.6 Appendix

6.6.1 Orthogonal polynomials

Orthogonal polynomials are classes of polynomials $\{p_n(x)\}$ defined over a range $[a, b]$ that obey an orthogonality relation:

$$\int_a^b \omega(x)\, p_m(x)\, p_n(x)\, dx = \delta_{mn} c_n \,, \tag{6.55}$$

where $\omega(x)$ is a weighting function and δ_{mn} is the Kronecker delta. If $c_n = 1$, then the polynomials are not only orthogonal, but orthonormal.

Orthogonal polynomials have very useful properties in the solution of mathematical and physical problems. Just as Fourier series provide a convenient method of expanding a periodic function in a series of linearly independent terms, orthogonal polynomials provide a natural way to solve, expand, and interpret solutions to many types of important differential equations. Orthogonal polynomials are especially easy to generate using Gram–Schmidt orthonormalization.

A list of common orthogonal polynomials is given in Table 6.6, where $\omega(x)$ is the weighting function and

$$c_n = \int_a^b \omega(x)[p_n(x)]^2 dx \,. \tag{6.56}$$

Table 6.6: The most popular orthogonal polynomials.

Polynomial	*Interval*	*Weight* $\omega(x)$	c_n
Legendre	$[-1, 1]$	1	$\frac{2}{2n+1}$
Laguerre	$[0, \infty]$	e^{-x}	1
Hermite	$[-\infty, \infty]$	e^{-x^2}	$\sqrt{\pi}2^n n!$
Chebyshev polynomial of the first kind	$[-1, 1]$	$(1-x^2)^{-1/2}$	$\begin{cases} \pi & \text{for } n = 0 \\ \pi/2 & \text{otherwise} \end{cases}$

The roots of orthogonal polynomials possess many useful properties. For instance, let $x_1 < x_2 < \ldots < x_n$ be the roots of the $p_n(x)$ with $x_0 = a$ and $x_n = b$. Then each interval $[x_\nu, x_{\nu+1}]$ for $\nu = 0, 1, \ldots, n$ contains exactly one root of $p_{n+1}(x)$. And between two roots of $p_n(x)$ there is at least one root of $p_m(x)$ for $m > n$.

Legendre polynomials

They are solutions $y = P_n(x)$ of the differential equation

$$(1+x^2)y'' - 2xy' + (n+1)ny = 0 \tag{6.57}$$

and satisfy the recurrence relation

$$P_n(x) = \frac{2n-1}{n}\, P_{n-1}(x) - \frac{(n-1)}{n}\, P_{n-2}(x) \tag{6.58}$$

with

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = \frac{1}{2}(3x^2 - 1), \quad \ldots \tag{6.59}$$

Chebyshev Polynomials (of the first kind)

They are solutions $y = T_n(x)$ of the differential equation

$$(1-x^2)y'' - xy' + n^2 y = 0 \tag{6.60}$$

and satisfy the recursion

$$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x) \tag{6.61}$$

with

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_2(x) = 2x^2 - 1, \quad \ldots \tag{6.62}$$

Hermite polynomials

They are solutions $y = H_n(x)$ of the differential equation

$$y'' - 2xy' + 2ny = 0 \tag{6.63}$$

and satisfy the recurrence relation

$$H_n(x) = 2xH_{n-1}(x) - 2(n-1)H_{n-2}(x) \tag{6.64}$$

with

$$H_0(x) = 1, \quad H_1(x) = 2x, \quad H_2(x) = 4x^2 - 2, \quad \ldots \tag{6.65}$$

Laguerre polynomials

They are solutions $y = L_n(x)$ of the differential equation

$$xy''(1-x)y' + ny = 0 \tag{6.66}$$

and satisfy the recurrence relation

$$L_n(x) = (2n-x-1)L_{n-1}(x) - (n-1)^2 L_{n-2}(x) \tag{6.67}$$

with

$$L_0(x) = 1, \quad L_1(x) = 1 - x, \quad L_2(x) = 2 - 4x + x^2, \quad \ldots \tag{6.68}$$

6.6.2 Expansion of an arbitrary polynomial in terms of orthogonal polynomials

An arbitrary polynomial $q_n(x)$ has a unique expansion in terms of any given family of orthogonal polynomials. Let

$$q_n(x) = \alpha_0 + \alpha_1 x + \ldots + \alpha_n x^n \tag{6.69}$$
$$= \beta_0\phi_0 + \beta_1\phi_1 + \ldots + \beta_n\phi_n\ . \tag{6.70}$$

For example let us express $q_2(x) = -2x^2 + 2x + 1$ in terms of *Legendre polynomials*. To do so we write

$$q_2(x) = \beta_0 P_0(x) + \beta_1 P_1(x) + \beta_2 P_2(x) \tag{6.71}$$
$$= \beta_0 + \beta_1 x + \beta_2 \frac{1}{2}(3x^2 - 1) \tag{6.72}$$
$$= \left(\beta_0 - \frac{\beta_2}{2}\right) + \beta_1 x + \frac{3\beta_2}{2}x^2 \tag{6.73}$$

which allows us to derive $\beta_0 = 1/3$, $\beta_1 = 2$, and $\beta_2 = -4/3$. That is,

$$q_2(x) = \frac{1}{3}P_0(x) + 2P_1(x) - \frac{4}{3}P_2(x) \tag{6.74}$$