eqr438

An introduction to quadrature and other numerical integration techniques

M. Concepcion Ausin

Department of Mathematics

Facultade de Matemáticas, Campus de Elviña

Universidade da Coruña

15071 A Coruña, Spain

Phone: +34 981 167 000 (ext. 1318)

Fax: + 34 981 167 160

mausin@udc.es*

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Abstract

The objective in numerical integration is the approximation of a definite integral using numerical techniques. There are a large number of numerical integration methods in the literature and this article overviews some of the most common ones, namely, the Newton-Cotes formulas, including the trapezoidal and Simpson's rules, and the Gaussian quadrature. Different procedures are compared and illustrated with examples. Discussions about more advanced numerical integration procedures are also included.

1 Introduction

A numerical integration technique is an algorithm to calculate the numerical value of a definite integral,

$$\int_a^b f(x)\,dx \tag{1}$$

Numerical integration problems go back at least to Greek antiquity when e.g. the area of a circle was obtained by successively increasing the number of sides of an inscribed polygon. In the seventeen century, the invention of calculus originates a new development of the subject leading to the basic numerical integration rules. In the following centuries, the field becomes more sophisticated and, with the introduction of computers in the recent past, many classical and new algorithms have been implemented leading to very fast and accurate results. Consequently, there is a vast amount of relevant literature on solving numerical integration problems consisting of books, articles, software packages, etc. Some essential references are [1, 2, 3, 4, 5, 6].

Numerical integration is sometimes called quadrature. A quadrature rule is a numerical approximation of an integral using a weighted sum of some values of the integrand,

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} \omega_i f(x_i),$$

where $x_1, \ldots, x_n$ are the points or abscissas, usually chosen to be in the interval of integration, and $\omega_1, \ldots, \omega_n$ are the weights associated to these points.

The simplest quadrature rules are the Riemann sums. Given a set of ordered abscissas, $a = x_1 < x_2 < \ldots < x_n = b$, the left-handed Riemann sum is obtained with,

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n-1} h_i f(x_i),$$

where $h_i = (x_{i+1} - x_i)$, the length of the i-th interval between points. Observe that the area under the curve in the i-th interval is approximated by a rectangle of width h_i and height $f(x_i)$. Analogously, one can define the right-handed and midpoint Riemann sums by evaluating the function on the maximum or midpoint value, respectively, of each i-th interval. The Riemann sums are also known as rectangular rules because of the use of rectangles to approximate the integral.

The rest of this paper is organized as follows. Section 2 describes the Newton-Cotes formulas which are based on evaluating the integrand at a number of equally spaced points. Section 3 introduces the Gaussian quadrature rules where the abscissas are chosen optimally to give the most accurate approximations possible. This section also includes a numerical example comparing different approaches. Some comments on the extensions of the Gaussian quadrature are also included. Section 4 concludes with some discussion and remarks.

2 Newton-Cotes formulas

Assume that we divide the interval $[a, b]$ into n equally spaced points such that,

$$x_i = x_1 + ih, \qquad \text{for } i = 0, 1, \ldots, n-1,$$

where $x_1 = a$, $x_n = b$ and $h = (b-a)/n$. Let us denote $f_i = f(x_i)$, for $i = 1, \ldots, n$. The main idea in Newton-Cotes formulas is to approximate the function $f(x)$ using polynomials that pass through the points (x_i, f_i) and integrate them to approximate the integral from x_1 to x_n. Newton-Cotes formulas are of closed type when the end-points, x_1 and x_n, are included in the set of abscissas and they are called of open type when the end-points are not used to approximate the integral.

The basic closed Newton-Cotes formula is the trapezoidal rule which uses two points, x_1 and x_2, and approximates the function $f(x)$ on $[x_1, x_2]$ using a straight line joining (x_1, f_1) and (x_2, f_2). Then, the function is approximated by the following first order polynomial,

$$f(x) \approx \left(\frac{f_2 - f_1}{h}\right) x + \frac{x_2 f_1 - x_1 f_2}{h}.$$

This polynomial can be integrated to give the following approximation,

$$\int_{x_1}^{x_2} f(x)\, dx \approx \int_{x_2}^{x_2} \frac{f_2 - f_1}{h} x + \frac{x_2 f_1 - x_1 f_2}{h} dx = \frac{h}{2}(f_1 + f_2).$$

Observe that this is called the trapezoidal rule because the area under $f(x)$ is approximated by a trapezoid with bases f_1 and f_2 and height $h = (x_2 - x_1)$, see Figure 1. The error of this approximation can be shown to be given by, see e.g. [2],

$$E_T = -\frac{h^3}{12} f''(\xi),$$

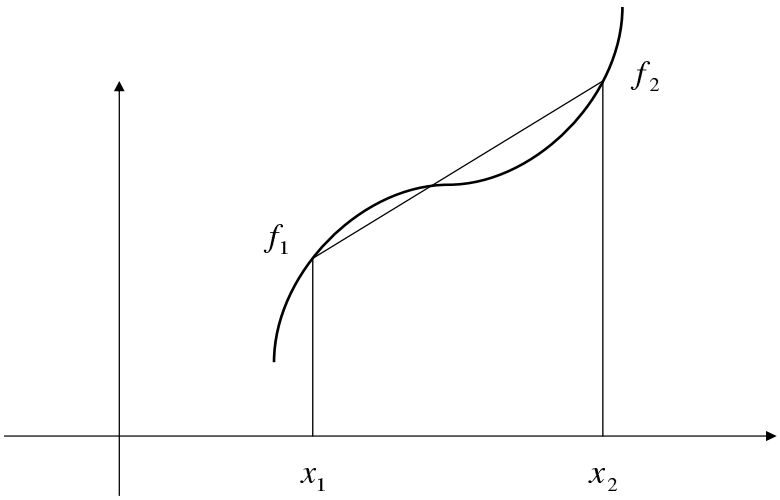

Figure 1: Trapezoidal rule

where ξ is some point in the interval $[x_1, x_2]$. Then, the amount of error will not be larger than the maximum value of the second derivative of the function in the interval and it will increase with the curvature of the function. The trapezoidal rule is exact for polynomials up to and including degree 1.

The trapezoidal rule can be used repeatedly to approximate the integral over the whole interval, $[x_1, x_n]$. This is called the extended or composite trapezoidal rule and is given by,

$$\begin{aligned}\int_{x_1}^{x_n} f(x)\,dx &= \int_{x_1}^{x_2} f(x)\,dx + ... + \int_{x_{n-1}}^{x_n} f(x)\,dx \\ &\approx h\left(\frac{f_1}{2} + f_2 + ... + f_{n-1} + \frac{f_n}{2}\right),\end{aligned}$$

whose approximation error is equal to $-(n-1)h^3 f''(\xi)/12$. A powerful extension of the trapezoidal rule is the Romberg integration, see e.g. [5], which uses a sequence of refinements of the extended trapezoidal rule by increasing carefully the number of subintervals.

The three-point closed Newton-Cotes formula is called the Simpson's rule and uses a

quadratic polynomial joining the points (x_1, f_1), (x_2, f_2) and (x_3, f_3) to approximate the function $f(x)$ on the interval $[x_1, x_3]$,

$$f(x) \approx \alpha x^2 + \beta x + \gamma,$$

where the coefficients α, β and γ are given by,

$$\begin{aligned}
\alpha &= \frac{f_1 - 2f_2 + f_3}{2h^2}, \\
\beta &= \frac{-2x_1(f_1 - 2f_2 + f_3) - h(3f_1 - 4f_2 + f_3)}{2h^2} \\
\gamma &= \frac{x_1^2(f_1 - 2f_2 + f_3) + hx_1(3f_1 - 4f_2 + f_3) + 2h^2 f_1}{2h^2}.
\end{aligned}$$

Then, we can integrate this second order polynomial to obtain the Simpson's approximation,

$$\int_{x_1}^{x_3} f(x)\,dx \approx \frac{h}{3}(f_1 + 4f_2 + f_3). \tag{2}$$

The error in this case can be shown to be given by,

$$E_S = -\frac{h^5}{90} f^{(iv)}(\xi), \tag{3}$$

where $f^{(iv)}(\xi)$ is the fourth derivative of $f(x)$ evaluated at some point ξ such that $x_1 \leq \xi \leq x_3$. Simpson's rule is exact for polynomials up to and including degree 3. This is surprising because it is designed to be exact for quadratic polynomials but, due to the symmetry of the formula, it is also exact for cubic polynomials.

As before, we can use the Simpson's rule repeatedly to obtain the following extended or composite Simpson's rule, where the number of points, n, must be odd,

$$\begin{aligned}
\int_{x_1}^{x_n} f(x)\,dx &= \int_{x_1}^{x_3} f(x)\,dx + ... + \int_{x_{n-2}}^{x_n} f(x)\,dx \\
&\approx \frac{h}{3}(f_1 + 4f_2 + 2f_3 + 4f_4 + 2f_5 ... + 4f_{n-1} + f_n).
\end{aligned} \tag{4}$$

The approximation error is equal to $-(n-1)h^5 f^{(iv)}(\xi)/180$. Note that the Simpson's rule will in general imply better accuracy than the trapezoidal rule if the function $f(x)$ is smooth enough (with finite fourth derivative).

The four-point closed Newton-Cotes formula is called the Simpson's 3/8 rule and is based on a cubic polynomial approximation,

$$f(x) \approx \alpha x^3 + \beta x^2 + \gamma x + \delta,$$

where α, β, γ and δ are constants such that the polynomial passes through the points $(x_1, f_1), \ldots, (x_4, f_4)$. These coefficients can be calculated using the Lagrange interpolation formulas, see e.g. [2]. Then, the Simpson's 3/8 rule can be obtained to be,

$$\int_{x_1}^{x_3} f(x)\, dx \approx \frac{3h}{8}\left(f_1 + 3f_2 + 3f_3 + f_4\right),$$

whose approximation error is given by,

$$E_{\tilde{S}} = -\frac{3h^5}{80} f^{(iv)}(\xi).$$

As expected, Simpson's 3/8 rule is exact for polynomials up to and including degree 3. Note that the approximation error for the Simpson's 3/8 rule is larger than the ordinary Simpson's error given in (3). However, the Simpson's 3/8 rule has the advantage that the number of points, n, is not required to be odd when it is used repeatedly to approximate the integral over the whole interval, $[x_1, x_n]$. Then, if n is even, one possibility is using 3/8 Simpson's rule for the first four points and the ordinary Simpson's rule for the remaining points, whose number (including the fourth point) is definitely odd.

The five-point closed Newton-Cotes formula is called the Boole's rule and is given by,

$$\int_{x_1}^{x_5} f(x)\,dx = \frac{2h}{45}\left(7f_1 + 32f_2 + 12f_3 + 32f_4 + 7f_5\right),$$

which can be obtained using the fourth order Lagrange polynomial that passes trough $(x_1, f_1), \ldots, (x_5, f_5)$. The error is $-8h^7 f^{(vi)}(\xi)/945$ and it is exact for polynomials of degree 5 or less. Boole's rule is also known as Bode's rule, as in e.g. [7], due to an early typo.

Further point closed Newton-Cotes formulas can be obtained by integrating the Lagrange polynomials that passes through the considered points, see e.g. [8]. In general, observe that higher point formulas will imply higher accuracy only when the function can be well approximated by a polynomial.

Open Newton-Cotes formulas approximate the integral from $a = x_1$ to $b = x_n$ without using the interior points, $x_2, x_2, ..., x_{n-1}$. Some of these formulas are shown in Table 1. Newton-Cotes formulas of open type can be useful for example when the function takes infinite values at the endpoints or when one or both endpoints are infinity. However, these are not very common in practice as it is not reasonable to use them repeatedly to obtain extended open rules. Also, the Gaussian quadrature rules, which will be described in the next section, lead always to more accurate approximations than open Newton-Cotes formulas.

3 Gaussian quadrature

Suppose now that we have the freedom to choose the abscissas at which to evaluate the function $f(x)$ rather than being equally spaced points. The Gaussian quadrature rules provide

Table 1: Newton-Cotes formulas of open type.

Approximation formula	Error
$\int_{x_1}^{x_3} f(x)\,dx \approx 2hf_2$	$\frac{h^3}{24} f''(\xi)$
$\int_{x_1}^{x_4} f(x)\,dx \approx \frac{3h}{2}(f_2 + f_3)$	$\frac{h^3}{4} f''(\xi)$
$\int_{x_1}^{x_5} f(x)\,dx \approx \frac{4h}{3}(2f_2 - f_3 + 2f_4)$	$\frac{28h^5}{90} f^{(iv)}(\xi)$
$\int_{x_1}^{x_6} f(x)\,dx \approx \frac{5h}{24}(11f_2 + f_3 + f_4 + 11f_5)$	$\frac{95h^5}{144} f^{(iv)}(\xi)$
$\int_{x_1}^{x_7} f(x)\,dx \approx \frac{6h}{20}(11f_2 - 14f_3 + 26f_4 - 14f_5 + 11f_6)$	$\frac{-41h^7}{140} f^{(vi)}(\xi)$

careful choices of these points in order to obtain much more accuracy in approximating the required integral. These are open formulas in the sense that it is not required to evaluate the function at the end-points. Furthermore, it is possible to define a weighting function, $W(x)$, such that the approximation of the integral will be exact for polynomials times this weight function instead of only for polynomials. Then, the numerical approximation will be as follows,

$$\int_a^b W(x) f(x)\,dx \approx \sum_{i=1}^{n} \omega_i f(x_i).$$

The advantage of incorporating a weighting function, $W(x)$, is that singularities or difficult terms can be removed from the function to be integrated.

An n-point Gaussian quadrature rule is constructed to be exact for polynomials of degree $(2n-1)$, by a suitable choice of the points, x_i, and weights, ω_i. In fact, it can be shown (see e.g. [5]) that the abscissas used for the n-point Gaussian quadrature formulas are optimal and given precisely by the roots of the n-th orthogonal polynomial, $p_n(x)$, for the same

interval, $[a,b]$, and weighting function, $W(x)$. A set of polynomials $\{p_n(x)\}$ is orthogonal if they satisfy the condition,

$$\int_a^b W(x)\, p_n(x)\, p_m(x)\, dx = 0, \qquad \text{for } n \neq m.$$

The simplest form of Gaussian quadrature uses uniform weighting, $W(x) = 1$, and the reference interval is $[a,b] = [-1,1]$. The orthogonal polynomials for this weighting function and interval are the Legendre polynomials, see e.g. [5], which are used to approximate the integrand $f(x)$ over the interval $[-1,+1]$ as follows,

$$\int_{-1}^{1} f(x)\, dx \approx \sum_{i=1}^{n} \omega_i f(x_i),$$

where x_i are the roots of the Legendre polynomials and ω_i are the corresponding weights, which are well-known for this case and are given in Table 2. If we are interested in approximating the integral defined on an arbitrary interval, $[a,b]$, we can use a simple change of variable as follows,

$$\int_a^b f(x)\, dx = k \int_{-1}^{1} f(c+kx)\, dx \approx k \sum_{i=1}^{n} \omega_i f(c+kx_i), \tag{5}$$

where $c = (b+a)/2$ and $k = (b-a)/2$. This is called the Gauss-Legendre quadrature rule. The following example illustrates and compares it with the Simpson's approximation.

Example Assume that we are interested in the approximation of the following integral,

$$\int_0^{\frac{\pi}{2}} \cos(x)\, dx,$$

Table 2: Gauss-Legendre abscissas and weights

n^o points	2	3		4		5		
x_i	$\pm\sqrt{\frac{1}{3}}$	0.0	$\pm$0.7746	$\pm$0.3399	$\pm$0.8611	0.0	$\pm$0.5385	$\pm$0.9062
ω_i	1.0	0.88889	0.55556	0.65215	0.34785	0.56889	0.47863	0.23693

which is known analytically to be one. Firstly, we use the two-point Gauss-Legendre quadrature, given in (5), to obtain the following approximation,

$$\int_0^{\frac{\pi}{2}} \cos(x)\, dx \approx \frac{\pi}{4}\left[1.0 \times \cos\left(\frac{\pi}{4} + \frac{\pi}{4\sqrt{3}}\right) + 1.0 \times \cos\left(\frac{\pi}{4} - \frac{\pi}{4\sqrt{3}}\right)\right] = 0.99847,$$

which is very close to the true value of one and gives an approximation error of 0.00153. Now, we approximate the same integral using the three-point Simpson's quadrature, given in (2),

$$\int_0^{\frac{\pi}{2}} \cos(x)\, dx \approx \frac{\pi}{12}\left[\cos(0) + 4\cos\left(\frac{\pi}{4}\right) + \cos\left(\frac{\pi}{2}\right)\right] = 1.0023.$$

This gives an approximation error of 0.0023 which is larger than the error obtained previously with the Gauss-Legendre quadrature that was based only on two points.

The Gaussian quadrature is also superior when it is compared with the composite Simpson's rule. For example, the four-point Gauss-Legendre quadrature gives the following approximation for the same integral,

$$\int_0^{\frac{\pi}{2}} \cos(x)\, dx \approx \frac{0.65215\pi}{4} \times \cos\left(\frac{\pi}{4} + \frac{0.3399\pi}{4}\right) + \frac{0.65215\pi}{4} \times \cos\left(\frac{\pi}{4} - \frac{0.3399\pi}{4}\right)$$
$$+ \frac{0.34785\pi}{4} \times \cos\left(\frac{\pi}{4} + \frac{0.8611\pi}{4}\right) + \frac{0.34785\pi}{4} \times \cos\left(\frac{\pi}{4} - \frac{0.8611\pi}{4}\right) = 0.999999977$$

which is a much better approximation than the obtained with the following composite Simpson's quadrature based on five points, as given in (4),

$$\int_0^{\frac{\pi}{2}} \cos(x)\,dx \approx \frac{\pi}{24}\cos(0) + 4\cos\left(\frac{\pi}{8}\right) + 2\cos\left(\frac{\pi}{4}\right) + 4\cos\left(\frac{3\pi}{8}\right) + \cos\left(\frac{\pi}{2}\right) = 1.000134585$$

Alternatively to the Gauss-Laguerre quadrature, other Gaussian rules can be developed using different classical orthogonal polynomials. Table 3 shows some of these polynomials together with their associated intervals and weighting functions. A large amount of information about these polynomials and their properties can be found in [7] and [9]. See also [5] and [10] for numerical procedures on the calculation of the abscissas and weights.

Table 3: Classical orthogonal polynomials with their intervals and weighting functions.

Interval	$W(x)$	Symbol	Polynomial
$[-1,1]$	1	$P_n(x)$	Legendre
$[0,\infty)$	e^{-x}	$L_n(x)$	Laguerre
$(-\infty,\infty)$	e^{-x^2}	$H_n(x)$	Hermite
$[-1,1]$	$(1-x^2)^{-1/2}$	$T_n(x)$	1^{st} kind Chebyshev
$[-1,1]$	$(1-x^2)^{1/2}$	$U_n(x)$	2^{nd} kind Chebyshev

When we have an unusual choice for $W(x)$, we can develop our own Gaussian quadrature although this task usually becomes more difficult. Firstly, we need to obtain the set of orthogonal polynomials for the considered interval and weighting function. This can be done for example using a recurrence relation as described in [5]. Then, we need to calculate

the zeros of these polynomials which will be the points, x_i, at which to evaluate the function. These can be obtained using a root-finding algorithm like Newton's method or faster procedures as the described in [5]. Finally, we need to calculate the weights ω_i which can be obtained analytically by integrating the orthogonal polynomials for which the approximation is exact. There are also alternative formulas which are more efficient for the calculation of these weights, see e.g. [5] and [10].

The Gaussian quadrature can be modified in order to incorporate one or both end-points in the set of abscissas, leading to the Radau and Lobatto quadrature formulas respectively, see e.g. [10]. These formulas use a uniform weighting function $W(x) = 1$ and the free abscissas are the roots of some polynomials related with the Legendre orthogonal polynomials. Radau and Lobatto quadratures are slightly less optimal than the Gaussian quadrature.

Another important extension of the Gaussian quadrature is the Gauss-Kronrod algorithm, see e.g. [5] and [10]. This is an adaptive Gaussian method where the abscissas are suitably selected such that they can be reused in the next iterations reducing the number of function evaluations. This approach is implemented in various software packages such as Mathematica (Wolfram Research Inc.).

4 Discussion and remarks

The generalization of the described quadrature rules to the multidimensional case is not straightforward. The main reason is that the number of function evaluations for an n-dimensional integral increases to the power of n and then, it becomes very expensive even for

low dimensional integrals. An alternative approach for these cases is the use of Monte Carlo integration (see eqr188, eqr456) which gives reasonable approximations for multidimensional integral defined over complicated regions.

It is frequent in practice to have a tabulated function at given points, x_i, obtained from experimental data. In these cases, the abscissas are predetermined and cannot be chosen at will. One possibility is to obtain the Lagrange polynomial which interpolates the observed points and integrate it to approximate the integral, see e.g. [10]. One alternative is the use of splines which are piecewise polynomial functions with some finite derivatives that can be arranged to interpolate the data points, see e.g. [2].

Finally, note that the problem of evaluating an integral such as the given in (1) is equivalent to solving the differential equation $y'(x) = f(x)$ with $y(a) = 0$. There are many numerical procedures in the literature for solving differential equations that could be applied for this problem, see e.g. [5]. These would be specially well suited when the function to integrate is concentrated around one or various peaks.

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