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An Elementary Approach to Quadrature Formulae

Mathematics

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ABSTRACT

Quadrature formulae or rules are used in the approximate evaluation of Integrals. This is an elegant and extremely useful branch of numerical analysis; even the most powerful methods are a ctually based on very simple mathematics. In this paper, we will examine the ideas behind a number of quadrature formulae.

Typically, the integrand is a complicated object, and the aim of the game is to obtain the most accurate estimate, with the minimum possible computation.

1.0 INTRODUCTION

Consider the integral

$$I = \int_a^b f(x)dx. \qquad 1$$

In view of the definition of integration, the most obvious means of estimating its value is to partition the interval [a, b] using the points.

$$a = x_0 < x_1 < \cdots < x_N = b \qquad 2$$

and then approximate the area between the graph of and the axis using rectangles, that is

$$I \approx \sum_{j=1}^{N} (x_j - x_{j-1}) f(x_j). \qquad 3$$

How might the approximation be improved? One possibility is to use more points ; another is to use trapezia instead of rectangles, in which case we have

$$I \approx \frac{1}{2} \sum_{j=1}^{N} (x_j - x_{j-1}) \big(f(x_j) + f(x_{j-1})\big) \qquad 4$$

that all but two of the evaluations that occur in (4) are used twice (the exceptions occurring at the end-points and), and so the total number of evaluations required is only one greater than for (3).

To obtain a still more accurate approximation, observe that (3) yields an exact result if is a constant, whereas the trapezium rule (4) is exact for any linear integrand. Therefore we might try constructing a formula that is exact for quadratic polynomials. To this end, let

$$\mathrm{P}(x) = A(x - x_j^*)^2 + B(x - x_j^*) + f(x_j^*), \qquad 5$$

Where x_j is the subinterval midpoint, i.e

$$x_j^* = \frac{x_j + x_{j-1}}{2} \qquad 6$$

Clearly P Next we choose so that the values of *P* and *f* coincide at two additional points, because then if is a polynomial of order two or less. Taking these points to be the subinterval ends and it is not difficult to show that

$$\mathrm{A} = \frac{2\,[f(x_j) - 2f + (x_j^*) + f(x_{j-1})]}{(x_j - x_{j-1})^2} \qquad 7$$

and

$$\mathrm{B} = \frac{f(x_j) - f(x_{j-1})}{x_j - x_{j-1}} \qquad 8$$

so,

$$\int_{x_{j-1}}^{x_j} f(x)dx \approx \int_{x_{j-1}}^{x_j} P(x)dx \qquad 9$$

and evaluating the integral on the right hand side yields

$$\int_{x_{j-1}}^{x_j} f(x)dx \approx \frac{x_j - x_{j-1}}{6} \times [f(x_j) + 4f(x_j^*) + f(x_{j-1})]. \qquad 10$$

This is Simpson's rule. Press, [1] explains that the derivation ensures an exact result for quadratic integrands, in fact Simpson's rule also integrates cubic polynomials exactly.

2.0 ERROR BOUNDS

What accuracy can we expect if we approximate the integral of an arbitrary function by that of a polynomial? Let represent the subinterval, and let be a polynomial of order whose coefficients are chosen so that for values of that lie within . Denote these values by and consider the function

$$F(x) = f(x) - P(x) + C(x - \alpha_0) \cdots (x - \alpha_n). \qquad 11$$

For any that is distinct from all of the , we can choose

$$\mathrm{C} = \frac{P(x^*) - f(x^*)}{(x^* - \alpha_0) \cdots (x^* - \alpha_n)}, \qquad 12$$

that in which case has distinct zeros for (x* and all of the . Then must have zeros, and by repeatedly applying the same reasoning (assuming that the required derivatives exist and are continuous), we conclude that must have at least one zero in , located at ., say. This value clearly depends on . Now is a polynomial of order so differentiating (11) times yields.

$$F^{(n+1)}(x) = f^{(n+1)}(x) + C(n+1)!, \qquad 13$$

hence C = Equating the two expressions that we now have for C, we find that

$$f(x^*) - P(x^*) = \frac{F^{(n+1)}(\xi(x^*))}{(n+1)!} (x^* - \alpha_0) \cdots (x^* - \alpha_n) \qquad 14$$

formula was obtained on the assumption that is distinct from the , but in fact both sides vanish when this is not the case, and so it is valid throughout *Ij*. Dropping the now superfluous asterisks, and integrating, we obtain

$$\int_{x_{j-1}}^{x_j} f(x)dx = \int_{x_{j-1}}^{x_j} P(x)dx + E \qquad 15$$

Where

$$E = \int_{x_{j-1}}^{x_j} \frac{f^{(n+1)}(\xi(x))}{(n+1)!} (x - \alpha_0) \cdots (x - \alpha_n) dx. \qquad 16$$

Integrating yields an point quadrature formula, as in the case of Simpson's rule, above. The extra term *E* is the error, but of course we don't know anything about , except that it lies in the interval *Ij*. For the simple case of the trapezium rule, we have

$$E = \frac{1}{2}\int_{x_{j-1}}^{x_j} f''(\xi(x))(x - x_{j-1})$$

$$(x - x_j)dx \qquad 17$$

the quadratic term in the integrand is of fixed sign. Hence,

$$|E| \le \frac{1}{2} \sup_{x\in I_j} |f''(x)|$$

$$\left|\int_{x_{j-1}}^{x_j} (x - x_{j-1})(x - x_j)dx\right|, \qquad 18$$

evaluating the integral yields

$$|E| \le \frac{(x_j - x_{j-1})^3}{12} \sup_{x\in I_j} |f''(x)| \qquad 19$$

We say that the error in the trapezium rule is of order three, due to the presence of the factor , which will be small if the partition (2) is sufficiently fine. For more complicated rules, obtaining the best possible bound on |E| tends to be quite involved. In any case, it is usually not possible to find a convenient bound for derivatives of particularly those of high order. Therefore results such as (19) are of limited usefulness, beyond determining the order of the error, which can be obtained much more easily, as we shall see. When no rigorous error bound is available, common practice is to compute two or more estimates of the integral under consideration. If these estimates are sufficiently close together, then we can have some confidence in their validity.

3.0 TAYLOR SERIES EXPANSIONS

The idea of designing quadrature formulae so as to exactly integrate polynomials points to a systematic approach to the overall problem, using Taylor series. To tidy the algebra, we make the substitution

$$x = \frac{(t+1)x_j}{2} - \frac{(t-1)x_{j-1}}{2},$$

$$-1 \le t \le 1, \qquad 20$$

in which case we have

$$\int_{x_{j-1}}^{x_j} f(x)dx = \frac{x_j - x_{j-1}}{2}\int_{-1}^{1} g(t)dt, \qquad 21$$

where

$$g(t) = f\left(\frac{(t+1)x_j}{2} - \frac{(t-1)x_{j-1}}{2}\right) \quad 22$$

Strictly, our subsequent analysis is valid for a quadrature rule with an order error if is times continuously differentiable on , but for the purposes of this article it is convenient to assume that the Taylor series

$$g(t) = \sum_{p=0}^{\infty} \frac{g^{(p)}(0)}{p!} t^p \qquad 23$$

converges for Integrating term by term, we obtain

$$\int_{-1}^{1} g(t)dt = \sum_{p=0}^{\infty} \frac{g^{(p)}(0)}{(p+1)!}$$

$$[1 + (-1)^p] \qquad 24$$

general, formulae for the derivatives of and therefore will not be available, so we cannot use this exact result directly. Instead, we use an approximation that requires values of itself; thus

$$\int_{-1}^{1} g(t)dt \approx \sum_{q=0}^{n} w_q g(t_q) \qquad 25$$

The points tq at which is evaluated are called abscissa, and the coefficients are called weights. Equations (3), (4) and (10) are all of this type. Subtracting (25) from (24) and using (23) with we find that the error in the approximation is given by

$$E = \sum_{p=0}^{\infty} \frac{g^{(p)}(0)}{p!} \left(\frac{1+(-1)^p}{p+1} \sum_{p=0}^{n} w_q t_q^p\right) 26$$

With this, Ueberhuber[3] can easily derive a number of different quadrature rules, by successively eliminating terms, starting with that in which p = 0. If we eliminate the first T terms from (26), then the lowest surviving derivative is , and since (21) provides an extra factor of we obtain a rule with an order T+1 error. A quadrature rule with an order T+1 error clearly integrates polynomials of order $T - 1$ exactly. Conversely, if we write.

$$g(t) = g_1(t) + g_2(t). \qquad 27$$

with

$$g_1(t) = \sum_{p=0}^{T-1} \frac{g^{(p)}(0)}{p!} t^p,$$

$$g_2(t) = \sum_{p=T}^{\infty} \frac{g^{(p)}(0)}{p!} t^p, \qquad 28$$

then, since the right-hand side of (25) is linear in g, it follows that formula which integrate polynomials of order $T - 1$ exactly has an error whose order is at least T +1.

4.0 METHODS

4.1 Newton – Cotes Quadrature

Newton-Cotes quadrature rules are characterized by the fact that the abscissa form a uniform partition of the integration range. Clearly this arrangement is symmetric about the midpoint of the range, which in the case of (25) is located at $t = 0$. Now we have n+1 free parameters (the weights , and so we should expect to be able to eliminate the terms with $p = 0$, 1, ...,n from (26). However, if we distribute the weights symmetrically as well, all of the terms in which p is odd will disappear. Thus, with a symmetric quadrature rule, and n+1 odd, the first nonzero term will be that in which $p = n+2$. Abramowite, et al[4], viewed another way, in order to maintain the symmetry that causes terms with p odd to vanish from (24), we must introduce pairs of equally weighted abscissae at
$t =$ with the exception of the abscissa at $t = 0$, which can be introduced alone. This is why Simpson's rule turned out to be better than we might have predicted. It is also the main reason why most of the widely used quadrature formulae have an odd number of abscissae.

In general, a symmetric quadrature formula with an odd number of abscissa has the form

$$\int_{-1}^{1} g(t)dt \approx$$

$$w_0 g(0) + \sum_{q=1}^{n} w_q \left[g(t_q) + g(-t_q)\right] \qquad 29$$

and using (23) and (24) yields the error

$$E = 2\sum_{p=0}^{\infty} \frac{g^{(2p)}(0)}{(2p)!}$$

$$\left(\frac{1}{2p+1} - \frac{w_0 \delta_{p0}}{2} - \sum_{q=1}^{n} w_q t_q^{2p}\right) \qquad 30$$

Here is the Kronecker delta, i.e 1 when $p = 0$ and 0 otherwise. Now in order to form a uniform partition, and we can eliminate n+1 terms using the free parameters Hence, the $(2n+1)$ point Newton-Cotes quadrature rule is obtained by solving the linear system.

$$\frac{1}{2p+1} - \frac{w_0 \delta_{p0}}{2} \sum_{q=1}^{n} w_q \left(\frac{q}{n}\right)^{2p} = 0,$$

$$p = 0, \dots, n. \qquad 31$$

If $n = 1$, then we have

$$1 - \frac{w_0}{2} - w_1 = 0, \text{ and } \frac{1}{3} - w_1 = 0. \quad 32$$

Solving retrieves Simpson's rule for the interval [-1,1], *i.e.*

$$\int_{-1}^{1} g(t)dt \approx \frac{1}{3}\,[g(-1) + 4g(0) + g(1)]. \qquad 33$$

This has an order five error.

Newton-Cotes formulae have the advantages that the calculated function values at the subinterval ends are used twice, with the exception of those at x=xo and $x = xN$ in (2). Further possibilities for the reuse of data arise if the partition (2) is refined, or if the integral in (21)is estimated using more than one quadrature rule.

4.2 GAUSSIAN QUADRATURE AND VARIANTS

Press, et al [5] explains that it can be advantageous for a quadrature rule to include an abscissa at the midpoint of the integration range. It turns out that there are other 'special' points, and

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finding these is the key to Gaussian quadrature. Thompson Ian [6], Consider the most general symmetric three-point quadrature rule, i.e (29) with *n*=1. This has three free parameters; the location of the abscissa and the weights and . If we attempt to eliminate the terms with *p = 0, p*=1 and *p* = 2 from (30), then we have

$$\left.\begin{aligned} 1 = \frac{w_0}{2} - \ w_1 = 0, \\ \frac{1}{3} - w_1 t_1^2 \quad = 0, \\ \frac{1}{5} - w_1 t_1^4 \ = 0, \end{aligned}\right\} \qquad 34$$

Immediately, we see that the last two equations are equivalent if we take 3/5. Then = 5/9 and = 8/9, leading to

$$\int_{-1}^{1} g(t)dt \approx \frac{1}{9}\left[5g(-\sqrt{3/5}+ 8g(0) + 5g\left(\sqrt{3/5}\right)\right]. \qquad 35$$

This is the three-point Gaussian quadrature formula. It has an order seven error, and is the most accurate three-point rule.

A minor drawback of Gaussian quadrature is that subinterval end-points are not used as abscissae and so no data is shared between consecutive subintervals, but this tends to be significantly outweighed by the extra orders of accuracy that Gaussian formulae offer over other methods. Of course, it is possible to create quadrature formulae in which the subinterval end-points are used, and the remaining abscissae are chosen so as to maximize accuracy. These are called Gauss-Lobatto rules, and, assuming symmetry and an odd number of points, they have the form (29), with = 1. The three-point Gauss-Lobatto rule is just Simpson's rule. With five abscissae, we have four free parameters; and . Setting the first four terms in (30) to zero yields.

$$\left.\begin{aligned} 1 = \frac{w_0}{2} - \ w_1 - w_2 = 0, \\ \frac{1}{3} - \ w_1 \ - w_2 t_2^2 \ = 0, \\ \frac{1}{5} - w_1 \ - w_2 t_2^4 \ = 0, \\ \frac{1}{7} - w_1 \ - w_2 t_2^6 \ = 0, \end{aligned}\right\} \qquad 36$$

Eliminating from the last two equations we obtain

$$\frac{2}{15} = w_2 t_2^2 (1 - t_2^2), \text{ and } \frac{2}{35} = w_2 t_2^4 (1 - t_2^2), \qquad 37$$

shows that setting = 3/7 introduces linear dependence. After solving for the weights, we obtain.

$$\int_{-1}^{1} g(t)dt \approx \frac{1}{90}[9g(-1) + 49g(-\sqrt{3/7} + 64g(0) + 49g\left(\sqrt{3/7}\right) + 9g(1)]. \qquad 38$$

This is the five-point Gauss-Lobatto rule. It allows for reuse of the end-point values of but has an order nine error, two orders lower than the 'pure' five-point Gaussian rule.

A more serious drawback of Gaussian formulae is that they are difficult to refine, because the locations of the abscissae change as they increase in number. Suppose that we have already computed our first estimate of an integral using the three-point Gaussian rule. What is the most efficient way in which we can reuse the data that we have, i.e and, and obtain in a more accurate approximation? If we add two further points, retaining symmetry, then we are free to choose three weights and one abscissa, and we might expect to obtain a rule with an order nine error in this way. Sadly, life is not that simple, as the nonlinear system of equations that results from inserting such a rule into (30) and setting the first four terms to zero turns out to have no solution. In fact, given the data required by the *n*-point Gaussian formula, *n*+1 additional points must be added in order to obtain a more accurate rule. This is called a Kronrod extension.

4.3 WEIGHTED QUADRATURE

Weighted quadrature is particularly useful for dealing with integrable singularities, and oscillatory functions, both of which impede the convergence of Taylor series. As an example, consider the integral.

$$I_m = \int_a^b f(x)\, e^{imx}\, dx, \quad m \in \mathbb{Z} \qquad 39$$

As |*m*/ increases, the integrand becomes highly oscillatory, and the accuracy of any formula based solely on polynomial approximation will deteriorate. This particular problem was originally considered by the fantastically named Louis Napoleon Goerge Filon [7] Once again, we divide the interval [a,b] using the partition (2), and then make the substitution (20) to obtain.

$$\int_{x_{j-1}}^{x_j} f(x)\, e^{imx}\, dx \frac{a}{m} e^{\frac{im(x_j + x_{j-1})}{2}} \int_{-1}^{1} g(t)\, e^{i\alpha t}\, dt, \qquad 40$$

where $g(t)$ is given by (22) and

$$\alpha = \frac{m(x_j + x_{j-1})}{2} \qquad 41$$

using the Taylor expansion (23), we find that

$$\int_{-1}^{1} g(t) e^{i\alpha t}\, dt = \sum_{p=0}^{\infty} \frac{g^{(p)}(0)}{p!} Q_p(\alpha). \qquad 42$$

Where

$$Q_p(\alpha) = \int_{-1}^{1} t^p e^{i\alpha t}\, dt \qquad 43$$

The exact value of this integral is

$$Q_p(\alpha) = \sum_{j=0}^{p} \frac{p!(i/\alpha)^{j+1}}{(p-j)!} \left[(-1)^{j+p} e^{-i\alpha} - e^{i\alpha}\right] \qquad 44$$

If we are dealing exclusively with the situation where /*α*/ is large, then the presence of removable singularities of α = 0 in (44) is of no concern. However, there are cases in which it is advantageous to simultaneously evaluate I*m* in (39) for a sequence of values of *m* (e.g. when calculating the coefficients in a Fourier series), and so we should not neglect the possibility that /*α*/ may be small. Thus, we note that expanding the exponential in (43) yields the alternative formula.

$$Q_p(\alpha) = \sum_{j=0}^{\infty} \frac{1 + (-1)^{p+j}}{j!(p+j+1)} (i\alpha)^j \qquad 45$$

which, from a computational point of view, is preferable to (44) when /*α*/ < 1.

Finally, we must obtain an approximation to the integral on the right-hand side of (40) that does not involve derivation of . To this end, we introduce the general *n*-point quadrature rule

$$\int_{-1}^{1} g(t) e^{i\alpha t}\, dt \approx \sum_{q=1}^{n} w_q\, g(t_q). \qquad 46$$

Then, we expand). Using (23), and compare the result to (42). In this way, we obtain the error

$$E = \sum_{p=0}^{\infty} \frac{g^{(p)}(0)}{p!} \left[Q_p(\alpha) - \sum_{q=1}^{n} w_q t_q^p\right] \qquad 47$$

If we attempt to optimize the locations of the abscissa, as in Gaussian quadrature, we will be forced to solve a nonlinear system for each value of . Since depends on the subinterval size and the parameter *m*, this is undesirable. Therefore we will use a uniform distribution, with (2q – *n* - 1) / (*n* - 1). In contrast to (24), the terms in (42) with *p* odd do not vanish in general, and so there are no longer any significant gains to be made by using an odd number of abscissa. Setting the first *n* equations in (47) to zero results in the linear system

$$\sum_{q=1}^{n} w_q \left(\frac{2q - n - 1}{n - 1}\right)^p = Q_p(\alpha), \quad p = 0, \ldots, n. \qquad 48$$

For a given number of abscissae, the matrix of known coefficients that appears on the left-hand side of this linear system need only be inverted once. The integrals *Qp* must be evaluated once for each value of *,* using either (44) or (45). The resulting Filon quadrature formulae can be used to accurately compute (39) with great efficiency, even when *(m)* is large.

5.0 Analysis of the methods

All of the methods discussed so far depend on the fact that the integrand can be well approximated (at least locally) by a polynomial. When this is not the case, we can expand as a series only that part of the integrand that is amenable to polynomial approximation, provided that the resulting expression can be integrated exactly. This is the key idea behind weighted quadrature formulae. The part of the integrand that is nor expanded is called the *weight function,* which is rather unfortunate terminology, as the word weight is now in use with two different meanings.

6.0 CONCLUSION

Most of the methods considered in this paper date back to the eighteenth and nineteenth centuries; a far more detailed discussion can be found in [8]. In particular, there are several weight functions for which the abscissa of Gaussian quadrature formulae are known, at least as roots of polynomials; again see [8] for details, Kronrod extensions are a more recent development [9]. The general problem of optimally extending quadrature formulae is considered in [10].

Perhaps the best way to get to grips with quadrature rules is to try them out. The basic formulae are easy to implement in any programming language with good mathematical features. Adaptive routines, which automatically adjust the partition (2) so as to achieve a desired level of accuracy, are slightly more difficult to write.

REFERENCE

[1] Press, W.H.; Flannery, B.P,; Teukolsky, S.A.; and Vetterling, W.T.(1992) | "Numerical Recipes in Fotran": The Art of Scientific computing | 2nd. Edition Cambridge, England: Cambridge University Press. | P. 154 | | [2] Nico, M.T.; (2010) "Section 3.5(V): Gauss Quadrature". Handbook of Cambridge University Press, England. | | [3] Ueberhuber, C.W. (1967). "Numerical Computation 2": Methods, Software and Analysis". Berlin, Springer – Verlag. pp. 105-106. | | [4] Abramowitz, M.; Stegun I.A.(1972) "Handbook of Mathematical Function" (with Formulas, Graphs and Mathematical Tables) P.888 | | [5] Press, W.H.; Teuskolsky, S.A.; Velterling, W.T.; Flannery, B.P. (2007), "Section 4.6 Graussian Quadratures and Orthogonal Polynomials." Numerical Recipes: The Art of scientific computing (Third Edition), Cambridge University Press, New York, USA | | [6] Thompson Ian, "Mathematics Today". (2010), vol.46, No.6, pp. 310-311. | | [7] Filon, L.N.G. (1929). "On a Quadrature Formula for Trigonometric Integrals". Proceedings of the Royal Society, Edinburgh, UK, vol.49, pp. 38-47 | | [8] Stoer, J.; Bulirsch R; (2002). "Introduction to Numerical Analysis". (Third Edition); Springer. pp. 172-175 | | [9] Rabinowitz, P. (1980). "The Exact Degree of Precision of Generalised Gauss-Kronrod Intergration rules". Mathematics of Computation. pp.1275-1283. | | [10] Patterson, T.N.L. (1968). The Optimum Addition of Points to Quadrature Formulae". Mathematics of Computation, vol.22, No.10, pp.847-856. |