Chapter D01

Quadrature

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1 Scope of the Chapter

This chapter provides routines for the numerical evaluation of definite integrals in one or more dimensions.

2 Background to the Problems

The routines in this chapter are designed to estimate:

(a) the value of a 1-d definite integral of the form

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

where $f(x)$ is defined by the user in the form of a function and the limits of integration a, b are finite.

Some methods are specially designed for integrands of the form

$$f(x) = w(x)g(x) \tag{2}$$

which contain a factor $w(x)$, called the weight-function, of a specific form. These methods take full account of any peculiar behaviour attributable to the $w(x)$ factor.

(b) the value of a multi-dimensional definite integral of the form

$$\int_{R_n} f(x_1, x_2, ..., x_n)\,dx_n ... dx_2\,dx_1, \tag{3}$$

where $f(x_1, x_2, ..., x_n)$ is a function defined by the user and R_n is some n-dimensional region.

The simplest form of R_n is the n-rectangle defined by

$$a_i \leq x_i \leq b_i, \quad i = 1, 2, ..., n, \tag{4}$$

where a_i and b_i are constants. When a_i and b_i are functions of x_j $(j < i)$, the region can easily be transformed to the rectangular form (see Davis and Rabinowitz [1] page 266). Some of the methods in this chapter incorporate the transformation procedure.

2.1 1-d Integrals

To estimate the value of a 1-d integral, a quadrature rule uses an approximation in the form of a weighted sum of integrand values, i.e.,

$$\int_a^b f(x)\,dx \simeq \sum_{i=1}^{N} w_i f(x_i). \tag{5}$$

The points x_i within the interval $[a, b]$ are known as the abscissae, and the w_i are known as the weights.

More generally, if the integrand has the form (2), the corresponding formula is

$$\int_a^b w(x)g(x)\,dx \simeq \sum_{i=1}^{N} w_i g(x_i). \tag{6}$$

If the functional form of the integrand is known, so that its value at any abscissa is easily obtained, then a wide variety of quadrature rules are available, each characterised by its choice of abscissae and the corresponding weights.

The appropriate rule to use will depend on the interval $[a, b]$ – whether finite or otherwise – and on the form of any $w(x)$ factor in the integrand. A suitable value of N depends on the general behaviour of $f(x)$; or of $g(x)$, if there is a $w(x)$ factor present. Currently, there are no procedures for treating integrals with infinite (or semi-finite) intervals in the Library.

Among possible rules, we mention particularly the Gaussian formulae, which employ a distribution of abscissae which is optimal for $f(x)$ or $g(x)$ of polynomial form.

The choice of basic rules constitutes one of the principles on which methods for 1-d integrals may be classified. The other major basis of classification is the implementation strategy, of which some types are now presented.

(a) **Single-rule evaluation procedures**

A fixed number of abscissae, N, is used. This number and the particular rule chosen uniquely determine the weights and abscissae. No estimate is made of the accuracy of the result. There are no procedures of this type currently included in the Library.

(b) **Automatic procedures**

The number of abscissae, N, within $[a, b]$ is gradually increased until consistency is achieved to within a level of accuracy (absolute or relative) requested by the user. There are essentially two ways of doing this; hybrid forms of these two methods are also possible:

(i) whole interval procedures (non-adaptive)

A series of rules using increasing values of N are successively applied over the whole interval $[a, b]$. It is clearly more economical if abscissae already used for a lower value of N can be used again as part of a higher-order formula. This principle is known as **optimal extension**. There is no overlap between the abscissae used in Gaussian formulae of different orders. However, the Kronrod formulae are designed to give an optimal $(2N + 1)$-point formula by adding $(N + 1)$ points to an N-point Gauss formula. Further extensions have been developed by Patterson. There are no procedures of this type currently included in the Library.

(ii) adaptive procedures

The interval $[a, b]$ is repeatedly divided into a number of sub-intervals, and integration rules are applied separately to each sub-interval. Typically, the subdivision process will be carried further in the neighbourhood of a sharp peak in the integrand than where the curve is smooth. Thus, the distribution of abscissae is adapted to the shape of the integrand. Automatic extrapolation over several levels of subdivision may eliminate the effects of some types of singularities.

Subdivision raises the problem of what constitutes an acceptable accuracy in each sub-interval. The usual **global acceptability criterion** demands that the sum of the absolute values of the error estimates in the sub-intervals should meet the conditions required of the error over the whole interval.

An ideal general-purpose method would be an automatic method which could be used for a wide variety of integrands, was efficient (i.e., required the use of as few abscissae as possible), and was reliable (i.e., always gave results within the requested accuracy). Complete reliability is unobtainable, and generally higher reliability is obtained at the expense of efficiency, and vice versa. **It must therefore be emphasised that the automatic routines in this chapter cannot be assumed to be 100% reliable. In general, however, the reliability is very high.**

2.2 Multi-dimensional Integrals

A distinction must be made between cases of moderately low dimensionality (say, up to 4 or 5 dimensions), and those of higher dimensionality. Where the number of dimensions is limited, a 1-d method may be applied to each dimension, according to some suitable strategy, and high accuracy may be obtainable (using product rules). However, the number of integrand evaluations rises very rapidly with the number of dimensions, so that the accuracy obtainable with an acceptable amount of computational labour is limited; for example, a product of 3-point rules in 20 dimensions would require more than 10^9 integrand evaluations. Special techniques such as the Monte Carlo, number theoretic, Sag–Szekeres and automatic adaptive methods can be used to deal with high dimensions. The routines in this chapter use a product integration rule for 2-d integrals and number theoretic as well as automatic adaptive methods for multi-dimensional integrals. For other special techniques such as the Monte Carlo and Sag–Szekeres methods which can be used to deal with high dimensions see Davis and Rabinowitz [1].

(a) **Products of 1-d rules**

Using a 2-d integral as an example, we have

$$\int_{a_1}^{b_1} \int_{a_2}^{b_2} f(x, y)\, dy\, dx \simeq \sum_{i=1}^{N} w_i \left(\int_{a_2}^{b_2} f(x_i, y)\, dy \right) \tag{7}$$

$$\int_{a_1}^{b_1}\int_{a_2}^{b_2} f(x,y)\,dy\,dx \simeq \sum_{i=1}^{N}\sum_{j=1}^{N} w_i v_j f(x_i,y_j) \tag{8}$$

where (w_i, x_i) and (v_i, y_i) are the weights and abscissae of the rules used in the respective dimensions.

A different 1-d rule may be used for each dimension, as appropriate to the range and any weight function present, and a different strategy may be used, as appropriate to the integrand behaviour as a function of each independent variable.

For a rule-evaluation strategy in all dimensions, the formula (8) is applied in a straightforward manner. For automatic strategies (i.e., attempting to attain a requested accuracy), there is a problem in deciding what accuracy must be requested in the inner integral(s). Reference to formula (7) shows that the presence of a limited but random error in the y-integration for different values of x_i can produce a 'jagged' function of x, which may be difficult to integrate to the desired accuracy, and for this reason products of automatic 1-d routines should be used with caution (see also Lyness [3]).

(b) **Number theoretic methods**

These are based on the work of Korobov and Conroy and operate by exploiting implicitly the properties of the Fourier expansion of the integrand. Special rules, constructed from so-called optimal coefficients, give a particularly uniform distribution of the points throughout the n-cube and from their number theoretic properties minimize the error on a prescribed class of integrals. The method can be combined with the Monte Carlo procedure.

(c) **Automatic adaptive procedures**

An automatic adaptive strategy in several dimensions normally involves division of the region into subregions, concentrating the divisions in those parts of the region where the integrand is worst behaved. It is difficult to arrange with any generality for variable limits in the inner integral(s). For this reason, some methods use a region where all the limits are constants; this is called a hyper-rectangle. Integrals over regions defined by variable or infinite limits may be handled by transformation to a hyper-rectangle. Integrals over regions so irregular that such a transformation is not feasible may be handled by surrounding the region by an appropriate hyper-rectangle and defining the integrand to be zero outside the desired region. Such a technique should always be followed by a Monte Carlo method for integration.

The method used locally in each subregion produced by the adaptive subdivision process is usually one of three types: Monte Carlo, number theoretic or deterministic. Deterministic methods are usually the most rapidly convergent but are often expensive to use for high dimensionality and not as robust as the other techniques.

2.3 References

[1] Davis P J and Rabinowitz P (1975) *Methods of Numerical Integration* Academic Press

[2] Gladwell I (1986) Vectorisation of one dimensional quadrature codes *Numerical Integration: Recent Developments, and Applications* (ed P Keast and G Fairweather) D Reidel Publishing Company, Holland 231–238

[3] Lyness J N (1983) When not to use an automatic quadrature routine *SIAM Rev.* **25** 63–87

[4] Piessens R, De Doncker-Kapenga E, Überhuber C and Kahaner D (1983) *QUADPACK, A Subroutine Package for Automatic Integration* Springer-Verlag

3 Recommendations on Choice and Use of Available Routines

Note: Refer to the Users' Note for your implementation to check that a routine is available.

3.1 1-d integrals

If the functional form of $f(x)$ is known, then one of the following approaches should be taken. They are arranged in the order from most specific to most general, hence the first applicable procedure in the list will be the most efficient. **However, if the user does not wish to make any assumptions about the integrand, the most reliable routine to use will be D01ATFP, although it will in general be less efficient for simple integrals.**

Automatic adaptive routines

Routine D01AXFP is available for integrands of the form $w(x)g(x)$, where $w(x)$ is a weight function of the form $w(x) = \cos(\omega x)$ or $\sin(\omega x)$ (this routine can also handle certain types of singularities in $g(x)$).

There are two routines for general $f(x)$. If $f(x)$ is known to be free of singularities, and possibly be oscillatory, D01AUFP may be used.

The most powerful of the finite interval integration routines is D01ATFP (which can cope with singularities of several types). It may be used if none of the more specific situations described above applies. D01ATFP is reliable for those integrands which have singularities, or discontinuities or cusps, and is therefore recommended where the integrand is known to be badly behaved, or where its nature is completely unknown.

The routines in this Chapter require the user to supply a subroutine to evaluate the integrand at an array of points. This approach can result in a shorter execution time than for those routines which require a function to be supplied for the evaluation of the integrand at a single point, especially on vector-processing machines (see Gladwell [2]).

3.2 Multi-dimensional Integrals

Three routines are available in this area.

(a) **Products of 1-d rules**

One routine is based on this method.

D01DAFP For 2-d integrals, unless the integrand is very badly behaved, the automatic whole-interval product procedure of this routine may be used. The limits of the inner integral may be user-specified functions of the outer variable. Infinite limits may be handled by transformation; end-point singularities introduced by transformation should not be troublesome, as the integrand value will not be required on the boundary of the region.

(b) **Number theoretic method**

One routine is based on this method.

D01GCFP carries out multiple integration using the Korobov–Conroy method over a product region with built-in transformation to the n-cube. A stochastic modification of this method is incorporated hybridising the technique with the Monte Carlo procedure. An error estimate is provided in terms of the statistical standard error. The routine includes a number of optimal coefficient rules for up to 20 dimensions. This method is suitable for high-dimensional integrals although the accuracy is not high.

(c) **Automatic routines**

One routine is based on this technique which is suitable for integrals of the form

$$\int_{a_1}^{b_1}\int_{a_2}^{b_2}\ldots\int_{a_n}^{b_n} f(x_1,x_2,\ldots,x_n)\,dx_n\,dx_{n-1}\,\ldots\,dx_1.$$

D01FAFP is an adaptive deterministic routine. Convergence is fast for well behaved integrands. Highly accurate results can often be obtained for n between 2 and 5. The routine will usually work when the integrand is mildly singular or oscillatory and $n \leq 10$.