NAG Library Chapter Introduction

d01 – Quadrature

Contents

1 Scope of the Chapter

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

2 Background to the Problems

The functions in this chapter are designed to estimate:

(a) the value of a one-dimensional definite integral of the form

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

where $f(x)$ is defined by you, either at a set of points $(x_i, f(x_i))$, for $i = 1, 2, \ldots, n$, where $a = x_1 < x_2 < \cdots < x_n = b$, or in the form of a function; and the limits of integration a, b may be finite or infinite.

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 values of the one-dimensional indefinite integrals arising from (1) where the ranges of integration are interior to the interval $[a, b]$.

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

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

where $f(x_1, x_2, \ldots, x_n)$ is a function defined by you and R_n is some region of n-dimensional space.

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

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

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 page 266 of Davis and Rabinowitz (1975)). Some of the methods described incorporate the transformation procedure.

2.1 One-dimensional Integrals

To estimate the value of a one-dimensional 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 integrand is known only at a fixed set of points, these points must be used as the abscissae, and the weighted sum is calculated using finite-difference methods. However, 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.

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 one-dimensional 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.

(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 you. 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.

(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.

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. Automatic extrapolation over several levels of subdivision may eliminate the effects of some types of singularities.

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 to 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 functions 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 one-dimensional 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 methods can be used to deal with high dimensions.

(a) Products of one-dimensional rules

Using a two-dimensional 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 one-dimensional 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 one-dimensional functions should be used with caution (see Lyness (1983)).

(b) Monte Carlo methods

These are based on estimating the mean value of the integrand sampled at points chosen from an appropriate statistical distribution function. Usually a variance reducing procedure is incorporated to combat the fundamentally slow rate of convergence of the rudimentary form of the technique. These methods can be effective by comparison with alternative methods when the integrand contains singularities or is erratic in some way, but they are of quite limited accuracy.

(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.

3 Recommendations on Choice and Use of Available Functions

The following three sub-sections consider in turn functions for: one-dimensional integrals over a finite interval, and over a semi-infinite or an infinite interval; and multi-dimensional integrals. Within each sub-section, functions are classified by the type of method, which ranges from simple rule evaluation to automatic adaptive algorithms. The recommendations apply particularly when the primary objective is simply to compute the value of one or more integrals, and in these cases the automatic adaptive functions are generally the most convenient and reliable, although also the most expensive in computing time.

Note however that in some circumstances it may be counter-productive to use an automatic function. If the results of the quadrature are to be used in turn as input to a further computation (e.g., an 'outer' quadrature or an optimization problem), then this further computation may be adversely affected by the 'jagged performance profile' of an automatic function; a simple rule-evaluation function may provide much better overall performance. For further guidance, the article by Lyness (1983) is recommended.

3.1 One-dimensional Integrals over a Finite Interval

(a) Integrand defined at a set of points

If $f(x)$ is defined numerically at four or more points, then the Gill–Miller finite difference method (nag_1d_quad_vals (d01gac)) should be used. The interval of integration is taken to coincide with the range of x values of the points supplied. It is in the nature of this problem that any function may be unreliable. In order to check results independently and so as to provide an alternative technique you may fit the integrand by Chebyshev series using nag_1d_cheb_fit (e02adc) and then use functions nag_1d_cheb_intg (e02ajc) and nag_1d_cheb_eval2 (e02akc) to evaluate its integral (which need not be restricted to the range of the integration points, as is the case for nag_1d_quad_vals (d01gac)). A further alternative is to fit a cubic spline to the data using nag_1d_spline_fit_knots (e02bac) and then to evaluate its integral using nag_1d_spline_intg (e02bdc).

(b) Integrand defined as a function

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 you do not wish to make any assumptions about the integrand, the most reliable functions to use will be nag_1d_quad_gen_1 (d01sjc).**

(i) Rule-evaluation functions

If $f(x)$ is known to be sufficiently well behaved (more precisely, can be closely approximated by a polynomial of moderate degree), a Gaussian function with a suitable number of abscissae may be used.

nag_1d_quad_gauss_1 (d01tac) may be used if it is not required to examine the weights and abscissae.

(ii) Automatic adaptive functions

Firstly, several functions are available for integrands of the form $w(x)g(x)$ where $g(x)$ is a 'smooth' function (i.e., has no singularities, sharp peaks or violent oscillations in the interval of integration) and $w(x)$ is a weight function of one of the following forms.

1. if $w(x) = (b-x)^{\alpha}(x-a)^{\beta}(\log(b-x))^{k}(\log(x-a))^{l}$, where $k, l = 0$ or 1, $\alpha, \beta > -1$: use nag_1d_quad_wt_alglog_1 (d01spc);
2. if $w(x) = \frac{1}{x-c}$: use nag_1d_quad_wt_cauchy_1 (d01sqc) (this integral is called the Hilbert transform of g);
3. if $w(x) = \cos(\omega x)$ or $\sin(\omega x)$: use nag_1d_quad_wt_trig (d01anc) (this function can also handle certain types of singularities in $g(x)$).

Secondly, there are some functions for general $f(x)$. If $f(x)$ is known to be free of singularities, though it may be oscillatory, nag_1d_quad_osc_1 (d01skc) may be used.

The most powerful of the finite interval integration functions is nag_1d_quad_gen_1 (d01sjc), which can cope with singularities of several types. It may be used if none of the more specific situations described above applies. nag_1d_quad_gen_1 (d01sjc) is somewhat more reliable, particularly where the integrand has singularities other than at an end point, or has discontinuities or cusps, and is therefore recommended where the integrand is known to be badly behaved, or where its nature is completely unknown.

Most of the functions in this chapter require you to supply a function or function to evaluate the integrand at a single point.

If $f(x)$ has singularities of certain types, discontinuities or sharp peaks **occurring at known points**, the integral should be evaluated separately over each of the subranges or nag_1d_quad_inf_wt_trig_1 (d01ssc) may be used.

3.2 One-dimensional Integrals over a Semi-infinite or Infinite Interval

(a) Integrand defined at a set of points

If $f(x)$ is defined numerically at four or more points, and the portion of the integral lying outside the range of the points supplied may be neglected, then the Gill–Miller finite difference method, nag_1d_quad_vals (d01gac), should be used.

(b) Integrand defined as a function

(i) Rule evaluation functions

If $f(x)$ behaves approximately like a polynomial in x, apart from a weight function of the form:

1. $e^{-\beta x}, \beta > 0$ (semi-infinite interval, lower limit finite); or
2. $e^{-\beta x}, \beta < 0$ (semi-infinite interval, upper limit finite); or
3. $e^{-\beta (x-\alpha)^2}, \beta > 0$ (infinite interval),

or if $f(x)$ behaves approximately like a polynomial in $(x+b)^{-1}$ (semi-infinite range), then the Gaussian functions may be used.

nag_1d_quad_gauss_1 (d01tac) may be used if it is not required to examine the weights and abscissae.

(ii) Automatic adaptive functions

nag_1d_quad_inf_1 (d01smc) may be used, except for integrands which decay slowly towards an infinite end point, and oscillate in sign over the entire range. For this class, it may be possible to calculate the integral by integrating between the zeros and invoking some extrapolation process.

nag_1d_quad_inf_wt_trig_1 (d01ssc) may be used for integrals involving weight functions of the form $\cos(\omega x)$ and $\sin(\omega x)$ over a semi-infinite interval (lower limit finite).

The following alternative procedures are mentioned for completeness, though their use will rarely be necessary.

1. If the integrand decays rapidly towards an infinite end point, a finite cut-off may be chosen, and the finite range methods applied.
2. If the only irregularities occur in the finite part (apart from a singularity at the finite limit, with which nag_1d_quad_inf_1 (d01smc) can cope), the range may be divided, with nag_1d_quad_inf_1 (d01smc) used on the infinite part.
3. A transformation to finite range may be employed,e.g.,

$$x = \frac{1-t}{t} \qquad \text{or} \qquad x = -\log_e t$$

will transform $(0,\infty)$ to $(1,0)$ while for infinite ranges we have

$$\int_{-\infty}^{\infty} f(x)\,dx = \int_0^{\infty} (f(x) + f(-x))\,dx.$$

If the integrand behaves badly on $(-\infty,0)$ and well on $(0,\infty)$ or vice versa it is better to compute it as $\int_{-\infty}^{0} f(x)\,dx + \int_0^{\infty} f(x)\,dx$. This saves computing unnecessary function values in the semi-infinite range where the function is well behaved.

3.3 Multi-dimensional Integrals

(a) Automatic functions (nag_multid_quad_adapt_1 (d01wcc) and nag_multid_quad_monte_carlo_1 (d01xbc))

Both functions are for integrals of the form

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

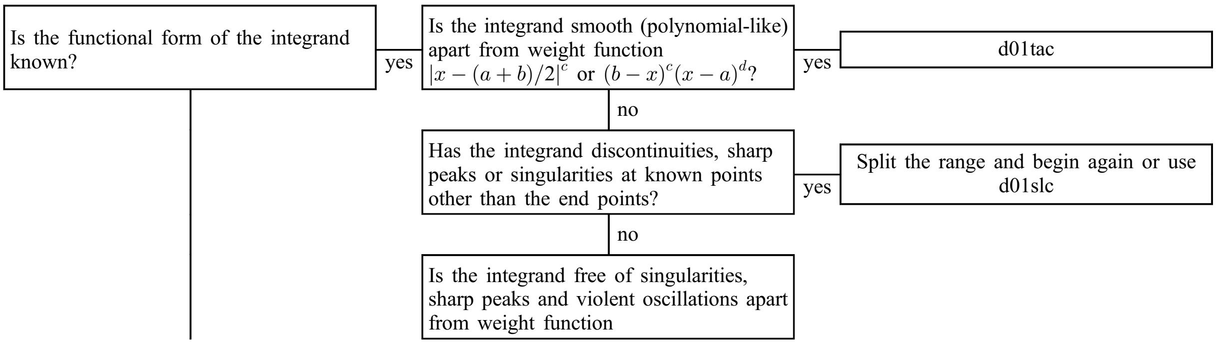
nag_multid_quad_monte_carlo_1 (d01xbc) is an adaptive Monte Carlo function. This function is usually slow and not recommended for high-accuracy work. It is a robust function that can often be used for low-accuracy results with highly irregular integrands or when n is large.

nag_multid_quad_adapt_1 (d01wcc) is an adaptive deterministic function. Convergence is fast for well behaved integrands. Highly accurate results can often be obtained for n between 2 and 5, using significantly fewer integrand evaluations than would be required by nag_multid_quad_monte_carlo_1 (d01xbc). The function will usually work when the integrand is mildly singular and for $n \leq 10$ should be used before nag_multid_quad_monte_carlo_1 (d01xbc). If it is known in advance that the integrand is highly irregular, it is best to compare results from at least two different functions.

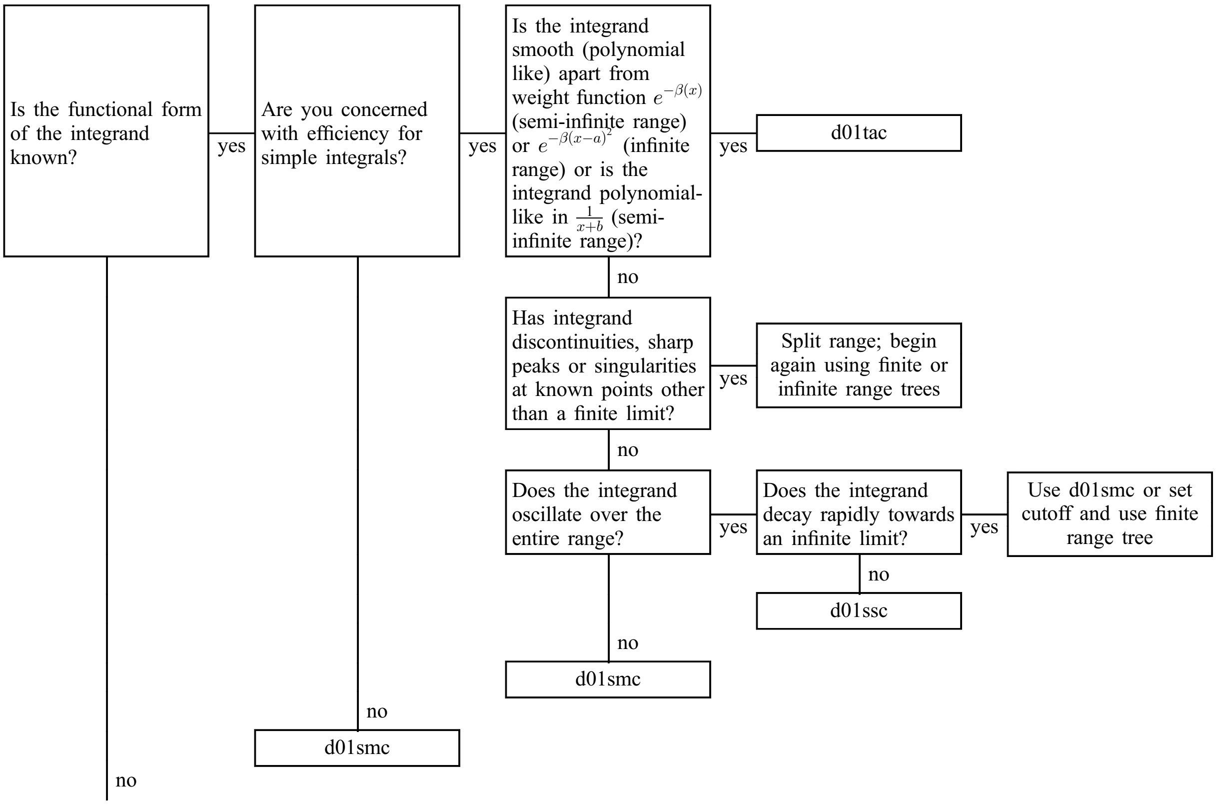
There are many problems for which one or both of the functions will require large amounts of computing time to obtain even moderately accurate results. The amount of computing time is controlled by the number of integrand evaluations allowed by you, and you should set this argument carefully, with reference to the time available and the accuracy desired.

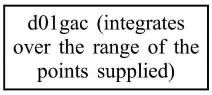
4 Decision Trees

Tree 1: One-dimensional integrals over a finite interval

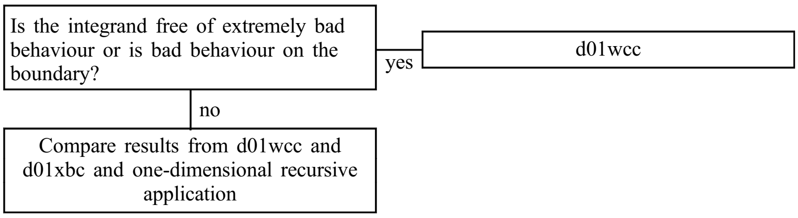


$(b-x)^{\alpha}(x-a)^{\beta}(\log(b-x))^{k}(\log(x-a))^{l}$? yes d01spc no Is the integrand free of singularities, sharp peaks and violent oscillations apart from weight function $\frac{1}{x-c}$? yes d01sqc no Is the integrand free of violent oscillations apart from weight function $\cos(\omega x)$ or $\sin(\omega x)$? yes d01snc no Is the integrand free of singularities? yes d01skc no d01sjc no d01gac **Tree 2: One-dimensional integrals over a semi-infinite or infinite interval**





Tree 3: Multi-dimensional integrals



5 Index

Multi-dimensional quadrature:
over a hyper-rectangle:
adaptive method, thread-safe .... nag_multid_quad_adapt_1 (d01wcc)
Monte Carlo method, thread-safe .... nag_multid_quad_monte_carlo_1 (d01xbc)

One-dimensional quadrature:
adaptive integration of a function over a finite interval:
allowing for singularities at user-specified break-points, thread-safe
.... nag_1d_quad_brkpts_1 (d01slc)
method suitable for oscillating functions, thread-safe .... nag_1d_quad_osc_1 (d01skc)
strategy due to Piessens and de Doncker,
allowing for badly behaved integrands, thread-safe .... nag_1d_quad_gen_1 (d01sjc)
weight function $1/(x-c)$ Cauchy principal value (Hilbert transform), thread-safe
.... nag_1d_quad_wt_cauchy_1 (d01sqc)
weight function with end-point singularities of algebraico-logarithmic type, thread-safe
.... nag_1d_quad_wt_alglog_1 (d01spc)
weight function $\cos(\omega x)$ or $\sin(\omega x)$ .... nag_1d_quad_wt_trig (d01anc)
weight function $\cos(\omega x)$ or $\sin(\omega x)$, thread-safe .... nag_1d_quad_wt_trig_1 (d01snc)
adaptive integration of a function over an infinite interval or semi-infinite interval, thread-safe
.... nag_1d_quad_inf_1 (d01smc)
adaptive integration of a function over an infinite interval or semi-infinite interval:
weight function $\cos(\omega x)$ or $\sin(\omega x)$, thread-safe .... nag_1d_quad_inf_wt_trig_1 (d01ssc)
Gaussian quadrature rule-evaluation, thread-safe .... nag_1d_quad_gauss_1 (d01tac)
integration of a function defined by data values only,
Gill–Miller method .... nag_1d_quad_vals (d01gac)

6 Functions Withdrawn or Scheduled for Withdrawal

Withdrawn Function	Mark of Withdrawal	Replacement Function(s)
nag_1d_quad_gen (d01ajc)	11	nag_1d_quad_gen_1 (d01sjc)
nag_1d_quad_osc (d01akc)	11	nag_1d_quad_osc_1 (d01skc)
nag_1d_quad_brkpts (d01alc)	11	nag_1d_quad_brkpts_1 (d01slc)
nag_1d_quad_inf (d01amc)	11	nag_1d_quad_inf_1 (d01smc)
nag_1d_quad_wt_alglog (d01apc)	11	nag_1d_quad_wt_alglog_1 (d01spc)
nag_1d_quad_wt_cauchy (d01aqc)	11	nag_1d_quad_wt_cauchy_1 (d01sqc)
nag_1d_quad_inf_wt_trig (d01asc)	11	nag_1d_quad_inf_wt_trig_1 (d01ssc)
nag_1d_quad_gauss (d01bac)	11	nag_1d_quad_gauss_1 (d01tac)
nag_multid_quad_adapt (d01fcc)	11	nag_multid_quad_adapt_1 (d01wcc)
nag_multid_quad_monte_carlo (d01gbc)	11	nag_multid_quad_monte_carlo_1 (d01xbc)

7 References

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

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

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

Piessens R, de Doncker–Kapenga E, Überhuber C and Kahaner D (1983) *QUADPACK, A Subroutine Package for Automatic Integration* Springer–Verlag

Sobol I M (1974) *The Monte Carlo Method* The University of Chicago Press

Stroud A H (1971) *Approximate Calculation of Multiple Integrals* Prentice–Hall