NAG Fortran Library Routine Document

D01AMF

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details.

1 Purpose

D01AMF calculates an approximation to the integral of a function $f(x)$ over an infinite or semi-infinite interval $[a, b]$:

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

2 Specification

```
SUBROUTINE D01AMF(F, BOUND, INF, EPSABS, EPSREL, RESULT, ABSERR, W, LW,
1                 IW, LIW, IFAIL)
INTEGER           INF, LW, IW(LIW), LIW, IFAIL
real              F, BOUND, EPSABS, EPSREL, RESULT, ABSERR, W(LW)
EXTERNAL          F
```

3 Description

D01AMF is based on the QUADPACK routine QAGI (Piessens *et al.* (1983)). The entire infinite integration range is first transformed to $[0, 1]$ using one of the identities:

$$\int_{-\infty}^{a} f(x)\,dx = \int_0^1 f\left(a - \frac{1-t}{t}\right)\frac{1}{t^2}\,dt$$

$$\int_{a}^{\infty} f(x)\,dx = \int_0^1 f\left(a + \frac{1-t}{t}\right)\frac{1}{t^2}\,dt$$

$$\int_{-\infty}^{\infty} f(x)\,dx = \int_0^{\infty} (f(x) + f(-x))\,dx = \int_0^1 \left[f\left(\frac{1-t}{t}\right) + f\left(\frac{-1+t}{t}\right)\right]\frac{1}{t^2}\,dt$$

where a represents a finite integration limit. An adaptive procedure, based on the Gauss 7-point and Kronrod 15-point rules, is then employed on the transformed integral. The algorithm, described by de Doncker (1978), incorporates a global acceptance criterion (as defined by Malcolm and Simpson (1976)) together with the ϵ-algorithm (Wynn (1956)) to perform extrapolation. The local error estimation is described by Piessens *et al.* (1983).

4 References

de Doncker E (1978) An adaptive extrapolation algorithm for automatic integration *ACM SIGNUM Newsl.* **13 (2)** 12–18

Malcolm M A and Simpson R B (1976) Local versus global strategies for adaptive quadrature *ACM Trans. Math. Software* **1** 129–146

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

Wynn P (1956) On a device for computing the $e_m(S_n)$ transformation *Math. Tables Aids Comput.* **10** 91–96

5 Parameters

1: F – ***real*** FUNCTION, supplied by the user. *External Procedure*

F must return the value of the integrand f at a given point.

Its specification is:

```
real FUNCTION F(X)
real             X
```

1: X – ***real*** *Input*

On entry: the point at which the integrand f must be evaluated.

F must be declared as EXTERNAL in the (sub)program from which D01AMF is called. Parameters denoted as *Input* must **not** be changed by this procedure.

2: BOUND – ***real*** *Input*

On entry: the finite limit of the integration range (if present). BOUND is not used if the interval is doubly infinite.

3: INF – INTEGER *Input*

On entry: indicates the kind of integration range:

if INF $=$ 1, the range is $[\text{BOUND}, +\infty)$

if INF $= -1$, the range is $(-\infty, \text{BOUND}]$

if INF $= +2$, the range is $(-\infty, +\infty)$.

Constraint: INF $= -1, 1$ or 2.

4: EPSABS – ***real*** *Input*

On entry: the absolute accuracy required. If EPSABS is negative, the absolute value is used. See Section 7.

5: EPSREL – ***real*** *Input*

On entry: the relative accuracy required. If EPSREL is negative, the absolute value is used. See Section 7.

6: RESULT – ***real*** *Output*

On exit: the approximation to the integral I.

7: ABSERR – ***real*** *Output*

On exit: an estimate of the modulus of the absolute error, which should be an upper bound for $|I - \text{RESULT}|$.

8: W(LW) – ***real*** array *Output*

On exit: details of the computation, as described in Section 8.

9: LW – INTEGER *Input*

On entry: the dimension of the array W as declared in the (sub)program from which D01AMF is called. The value of LW (together with that of LIW below) imposes a bound on the number of sub-intervals into which the interval of integration may be divided by the routine. The number of sub-intervals cannot exceed LW/4. The more difficult the integrand, the larger LW should be.

Suggested value: a value in the range 800 to 2000 is adequate for most problems.

Constraint: LW $\geq$ 4.

10: IW(LIW) – INTEGER array *Output*

On exit: IW(1) contains the actual number of sub-intervals used. The rest of the array is used as workspace.

11: LIW – INTEGER *Input*

On entry: the dimension of the array IW as declared in the (sub)program from which D01AMF is called. The number of sub-intervals into which the interval of integration may be divided cannot exceed LIW.

Suggested value: LIW = LW/4.

Constraint: LIW $\geq$ 1.

12: IFAIL – INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. Users who are unfamiliar with this parameter should refer to Chapter P01 for details.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, because for this routine the values of the output parameters may be useful even if IFAIL $\neq$ 0 on exit, the recommended value is -1. **When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.**

6 Error Indicators and Warnings

If on entry IFAIL = 0 or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

IFAIL = 1

The maximum number of subdivisions allowed with the given workspace has been reached, without the requested accuracy requirements being achieved. Look at the integrand in order to determine the integration difficulties. If the position of a local difficulty within the interval can be determined (e.g., a singularity of the integrand or its derivative, a peak, a discontinuity, etc.) you will probably gain from splitting up the interval at this point and calling D01AMF on the infinite subrange and an appropriate integrator on the finite subrange. Alternatively, consider relaxing the accuracy requirements specified by EPSABS and EPSREL, or increasing the amount of workspace.

IFAIL = 2

Round-off error prevents the requested tolerance from being achieved. The error may be underestimated. Consider requesting less accuracy.

IFAIL = 3

Extremely bad local integrand behaviour causes a very strong subdivision around one (or more) points of the interval. The same advice applies as in the case of IFAIL = 1.

IFAIL = 4

The requested tolerance cannot be achieved, because the extrapolation does not increase the accuracy satisfactorily; the returned result is the best which can be obtained. The same advice applies as in the case of IFAIL = 1.

IFAIL $= 5$

The integral is probably divergent, or slowly convergent. It must be noted that divergence can also occur with any other non-zero value of IFAIL.

IFAIL $= 6$

On entry, LW < 4,
or LIW < 1,
or INF $\neq -1, 1$ or 2.

7 Accuracy

The routine cannot guarantee, but in practice usually achieves, the following accuracy:

$$|I - \text{RESULT}| \leq tol,$$

where

$$tol = \max\{|\text{EPSABS}|, |\text{EPSREL}| \times |I|\},$$

and EPSABS and EPSREL are user-specified absolute and relative error tolerances. Moreover, it returns the quantity ABSERR, which, in normal circumstances, satisfies

$$|I - \text{RESULT}| \leq \text{ABSERR} \leq tol.$$

8 Further Comments

The time taken by the routine depends on the integrand and the accuracy required.

If IFAIL $\neq 0$ on exit, then the user may wish to examine the contents of the array W, which contains the end-points of the sub-intervals used by D01AMF along with the integral contributions and error estimates over these sub-intervals.

Specifically, for $i = 1, 2, \ldots, n$, let r_i denote the approximation to the value of the integral over the sub-interval $[a_i, b_i]$ in the partition of $[a, b]$ and e_i be the corresponding absolute error estimate. Then, $\int_{a_i}^{b_i} f(x)\,dx \simeq r_i$ and RESULT $= \sum_{i=1}^{n} r_i$ unless D01AMF terminates while testing for divergence of the integral (see Section 3.4.3 of Piessens *et al.* (1983)). In this case, RESULT (and ABSERR) are taken to be the values returned from the extrapolation process. The value of n is returned in IW(1), and the values a_i, b_i, e_i and r_i are stored consecutively in the array W, that is:

$$\begin{aligned} a_i &= \text{W}(i), \\ b_i &= \text{W}(n+i), \\ e_i &= \text{W}(2n+i) \text{ and} \\ r_i &= \text{W}(3n+i). \end{aligned}$$

Note: this information applies to the integral transformed to (0,1) as described in Section 3, not to the original integral.

9 Example

To compute

$$\int_0^\infty \frac{1}{(x+1)\sqrt{x}}\,dx.$$

The exact answer is π.

9.1 Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     D01AMF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          LW, LIW
      PARAMETER        (LW=800,LIW=LW/4)
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
*     .. Scalars in Common ..
      INTEGER          KOUNT
*     .. Local Scalars ..
      real             A, ABSERR, EPSABS, EPSREL, RESULT
      INTEGER          IFAIL, INF
*     .. Local Arrays ..
      real             W(LW)
      INTEGER          IW(LIW)
*     .. External Functions ..
      real             FST
      EXTERNAL         FST
*     .. External Subroutines ..
      EXTERNAL         D01AMF
*     .. Common blocks ..
      COMMON           /TELNUM/KOUNT
*     .. Executable Statements ..
      WRITE (NOUT,*) 'D01AMF Example Program Results'
      EPSABS = 0.0e0
      EPSREL = 1.0e-04
      A = 0.0e0
      INF = 1
      KOUNT = 0
      IFAIL = -1
*
      CALL D01AMF(FST,A,INF,EPSABS,EPSREL,RESULT,ABSERR,W,LW,IW,LIW,
     +            IFAIL)
*
      WRITE (NOUT,*)
      WRITE (NOUT,99999) 'A      - lower limit of integration = ', A
      WRITE (NOUT,*) 'B      - upper limit of integration = infinity'
      WRITE (NOUT,99998) 'EPSABS - absolute accuracy requested = ',
     +  EPSABS
      WRITE (NOUT,99998) 'EPSREL - relative accuracy requested = ',
     +  EPSREL
      WRITE (NOUT,*)
      IF (IFAIL.NE.0) WRITE (NOUT,99996) 'IFAIL = ', IFAIL
      IF (IFAIL.LE.5) THEN
         WRITE (NOUT,99997) 'RESULT - approximation to the integral = ',
     +     RESULT
         WRITE (NOUT,99998) 'ABSERR - estimate of the absolute error = '
     +     , ABSERR
         WRITE (NOUT,99996) 'KOUNT  - number of function evaluations = '
     +     , KOUNT
         WRITE (NOUT,99996) 'IW(1)  - number of subintervals used = ',
     +     IW(1)
      END IF
      STOP
*
99999 FORMAT (1X,A,F10.4)
99998 FORMAT (1X,A,e9.2)
99997 FORMAT (1X,A,F9.5)
99996 FORMAT (1X,A,I4)
      END
*
      real  FUNCTION FST(X)
*     .. Scalar Arguments ..
      real              X
*     .. Scalars in Common ..
```

```
      INTEGER           KOUNT
*     .. Intrinsic Functions ..
      INTRINSIC         SQRT
*     .. Common blocks ..
      COMMON            /TELNUM/KOUNT
*     .. Executable Statements ..
      KOUNT = KOUNT + 1
      FST = 1.0e0/((X+1.0e0)*SQRT(X))
      RETURN
      END
```

9.2 Program Data

None.

9.3 Program Results

```
 D01AMF Example Program Results

 A      - lower limit of integration =     0.0000
 B      - upper limit of integration = infinity
 EPSABS - absolute accuracy requested =  0.00E+00
 EPSREL - relative accuracy requested =  0.10E-03

 RESULT - approximation to the integral =   3.14159
 ABSERR - estimate of the absolute error =  0.27E-04
 KOUNT  - number of function evaluations =  285
 IW(1)  - number of subintervals used =   10
```