

1 SUMMARY

Given a **piecewise linear function** $S(x)$, defined by points $\xi_i, i=1,2,\dots,n$ and function values

$$S_i = S(\xi_i), \quad i=1,2,\dots,n, \quad n \geq 2$$

and given **integration limits** a and b , and **parameters** ϕ and \bar{x} the subroutine evaluates

$$Q(\phi, \bar{x}) = \int_a^b e^{-|\phi(x-\bar{x})|^2} S(x) dx$$

The subroutine can be applied to the problem of **folding a Gaussian into a function**.

ATTRIBUTES — **Version:** 1.0.0. **Types:** QG03A, QG03AD. **Calls:** FC07, FC08. **Original date:** May 1975. **Origin:** S.Marlow, Harwell.

2 HOW TO USE THE PACKAGE

2.1 Argument list and calling sequence

The single precision version

```
Q=QG03A(A,B,N,XI,S,PHI,XBAR)
```

The double precision version

```
DOUBLE PRECISION Q
-
-
Q=QG03AD(A,B,N,XI,S,PHI,XBAR)
```

The arguments

A, B are REAL (DOUBLE PRECISION in the D version) variables which must be set by the user to a and b the lower and upper limits of the integration respectively. If either a or b is outside the range ξ_1 to ξ_n the integral is calculated on the assumption that $S(x)=0$ for $x < \xi_1$ and $x > \xi_n$. If $a > b$ the sign of the integral is appropriately modified.

N is an INTEGER variable which must be set by the user to n the number of join points. **Restriction:** $n \geq 2$.

XI is a REAL (DOUBLE PRECISION in the D version) array of length at least n which must be set by the user to the join values $\xi_i, i=1,2,\dots,n$. The values must be ordered and distinct, i.e. $\xi_1 < \xi_2 < \dots < \xi_n$.

S is a REAL (DOUBLE PRECISION in the D version) array of length at least n which must be set by the user to the values of the linear function at the joins. $S_i = S(\xi_i), i=1,2,\dots,n$.

PHI is a REAL (DOUBLE PRECISION in the D version) variable which must be set by the user to the value of ϕ . Only the modulus of ϕ is used by the subroutine.

XBAR is a REAL (DOUBLE PRECISION in the D version) variable which must be set by the user to the value of \bar{x} .

Function value

QG03A and QG03AD are Fortran FUNCTION subroutines and will be set to the value of the integral on return.

2.2 Common block and diagnostic messages

The subroutine uses a common block which the user may also reference

The single precision version

```
COMMON/QG03B/ LP, IERR
```

The double precision version

```
COMMON/QG03BD/ LP, IERR
```

LP is an INTEGER variable (initial value = 6) and specifies the Fortran output unit to be used for diagnostic printing. LP may be reset by the user to any valid stream number. If LP is zero or negative printing is suppressed.

IERR is an INTEGER variable set by the subroutine to one of the following values:

0 successful entry to the subroutine.

-1 value of N was less than two.

>0 then IERR=i where $\xi_i > \xi_{i+1}$, that is the joins did not satisfy the original conditions.

3 GENERAL INFORMATION

Use of common: uses a common block called QG03B/BD, see §2.2.

Workspace: none.

Other routines called directly: FC07, FC08.

Input/output: diagnostic messages are printed, see §2.2.

Restrictions: $n \geq 2$, $\xi_1 < \xi_2 < \dots < \xi_n$.

4 METHOD

The subroutine first ensures that the limits a and b are sensible. The integral can be expressed as

$$\int_a^{x_j} f_{j-1}(x) dx + \sum_{i=j}^k \int_{x_i}^{x_{i+1}} f_i(x) dx + \int_{x_{k+1}}^b f_{k+1}(x) dx$$

or

$$\int_a^b f_i(x) dx$$

if both a and b are inside the same interval. Where $f_i(x)$, $i=j-1, \dots, k+1$ are of the form

$$S_i(x) e^{-\theta(x-\bar{x})^2}$$

and $S_i(x)$ are simple linear forms in x . Each of the integrals is reduced by integration by parts to an analytic function and a multiple of the integral

$$\int e^{-x^2} dx$$

between suitable limits. This integral is evaluated by using the error function or complementary error function, the choice being made to minimise loss of accuracy.