NAG Library Routine Document

D04BBF

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

D04BBF generates abscissae about a target abscissa x_0 for use in a subsequent call to D04BAF.

2 Specification

```
SUBROUTINE D04BBF (X_0, HBASE, XVAL)
REAL (KIND=nag_wp) X_0, HBASE, XVAL(21)
```

3 Description

D04BBF may be used to generate the necessary abscissae about a target abscissa x_0 for the calculation of derivatives using D04BAF.

For a given x_0 and h, the abscissae correspond to the set $\{x_0, x_0 \pm (2j-1)h\}$, for $j = 1, 2, \ldots, 10$. These 21 points will be returned in ascending order in XVAL. In particular, XVAL(11) will be equal to x_0.

4 References

Lyness J N and Moler C B (1969) Generalised Romberg methods for integrals of derivatives *Numer. Math.* **14** 1–14

5 Parameters

1:    X_0 – REAL (KIND=nag_wp)   *Input*

   On entry: the abscissa x_0 at which derivatives are required.

2:    HBASE – REAL (KIND=nag_wp)   *Input*

   On entry: the chosen step size h. If $h < 10\epsilon$, where $\epsilon = $ X02AJF(), then the default $h = \epsilon^{(1/4)}$ will be used.

3:    XVAL(21) – REAL (KIND=nag_wp) array   *Output*

   On exit: the abscissae for passing to D04BAF.

6 Error Indicators and Warnings

None.

7 Accuracy

Not applicable.

8 Parallelism and Performance

Not applicable.

9 Further Comments

The results computed by D04BAF depend very critically on the choice of the user-supplied step length h. The overall accuracy is diminished as h becomes small (because of the effect of round-off error) and as h becomes large (because the discretization error also becomes large). If the process of calculating derivatives is repeated four or five times with different values of h one can find a reasonably good value. A process in which the value of h is successively halved (or doubled) is usually quite effective. Experience has shown that in cases in which the Taylor series for for the objective function about x_0 has a finite radius of convergence R, the choices of $h > R/19$ are not likely to lead to good results. In this case some function values lie outside the circle of convergence.

10 Example

See Section 10 in D04BAF.