NAG Library Function Document

nag_numdiff_1d_real_absci (d04bbc)

1 Purpose

nag_numdiff_1d_real_absci (d04bbc) generates abscissae about a target abscissa x_0 for use in a subsequent call to nag_numdiff_1d_real_eval (d04bac).

2 Specification

```
#include <nag.h>
#include <nagd04.h>
```

```
void nag_numdiff_1d_real_absci (double x_0, double hbase, double xval[])
```

3 Description

nag_numdiff_1d_real_absci (d04bbc) may be used to generate the necessary abscissae about a target abscissa x_0 for the calculation of derivatives using nag_numdiff_1d_real_eval (d04bac).

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**[10] 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 Arguments

1: **x_0** – double *Input*

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

2: **hbase** – double *Input*

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

3: **xval**[**21**] – double *Output*

On exit: the abscissae for passing to nag_numdiff_1d_real_eval (d04bac).

6 Error Indicators and Warnings

None.

7 Accuracy

Not applicable.

8 Parallelism and Performance

nag_numdiff_1d_real_absci (d04bbc) is not threaded in any implementation.

9 Further Comments

The results computed by nag_numdiff_1d_real_eval (d04bac) 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 nag_numdiff_1d_real_eval (d04bac).