NAG Toolbox

nag_numdiff_sample (d04bb)

1 Purpose

nag_numdiff_sample (d04bb) generates abscissae about a target abscissa x_0 for use in a subsequent call to nag_numdiff_rcomm (d04ba).

2 Syntax

```
[xval] = nag_numdiff_sample(x_0, hbase)
[xval] = d04bb(x_0, hbase)
```

3 Description

nag_numdiff_sample (d04bb) may be used to generate the necessary abscissae about a target abscissa x_0 for the calculation of derivatives using nag_numdiff_rcomm (d04ba).

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

5.1 Compulsory Input Parameters

1: **x_0** – REAL (KIND=nag_wp)

The abscissa x_0 at which derivatives are required.

2: **hbase** – REAL (KIND=nag_wp)

The chosen step size h. If $h < 10\epsilon$, where $\epsilon =$ x02aj(), then the default $h = \epsilon^{(1/4)}$ will be used.

5.2 Optional Input Parameters

None.

5.3 Output Parameters

1: **xval**(**21**) – REAL (KIND=nag_wp) array

The abscissae for passing to nag_numdiff_rcomm (d04ba).

6 Error Indicators and Warnings

None.

7 Accuracy

Not applicable.

8 Further Comments

The results computed by nag_numdiff_rcomm (d04ba) 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.

9 Example

See Section 10 in nag_numdiff_rcomm (d04ba).

9.1 Program Text

```
function d04bb_example

fprintf('d04bb example results\n\n');

fprintf('\nFind the derivatives of the polygamma (psi) function\n');
fprintf('using function values generated by s14ae.\n\n');
fprintf('Demonstrate the effect of successively reducing hbase.\n\n');

% Set the target location and calculate the objective value
x_0 = 0.05;
[f_0, ifail] = s14ae(x_0, nag_int(0));

% Compute the actual derivatives using s14ae for comparison
actder = zeros(3, 1);
for j=1:3
  [actder(j), ifail] = s14ae(x_0, nag_int(j));
end

der_comp = zeros(14, 3, 4);
% Attempt 4 applications, reducing hbase by factor 0.1 each time
for j=1:4
  % Generate the abscissa xval using d04bb
  hbase = 0.025*10^(-j);
  [xval] = d04bb(x_0, hbase);

  % Calculate the corresponding objective function values
  fval(11) = f_0;
  for k=[1:10,12:21]
    [fval(k), ifail] = s14ae(xval(k), nag_int(0));
  end

  % Call d04ba to calculate the derivative estimates
  [der, erest, ifail] = d04ba(xval, fval);

  % Store results in der_comp
  der_comp(:, 1, j) = hbase;
  der_comp(:, 2, j) = der;
  der_comp(:, 3, j) = erest;

end

% Display results for first 3 derivatives
for i=1:3
  fprintf('\nderivative %d calculated using s14ae: %11.4e\n', i, actder(i));
  fprintf('Derivative and error estimates for derivative %d\n', i);
  fprintf('      hbase        der(%d)      erest(%d)\n', i, i);
  for j=1:4
    fprintf('  %12.4e %12.4e %12.4e\n', der_comp(i,:,j));
  end
end
```

9.2 Program Results

```
     d04bb example results

Find the derivatives of the polygamma (psi) function
using function values generated by s14ae.

Demonstrate the effect of successively reducing hbase.

derivative 1 calculated using s14ae:  4.0153e+02
Derivative and error estimates for derivative 1
      hbase        der(1)      erest(1)
    2.5000e-03   4.0204e+02   1.3940e+02
    2.5000e-04   4.0153e+02   4.9170e-11
    2.5000e-05   4.0153e+02   2.1799e-10
    2.5000e-06   4.0153e+02   1.1826e-09

derivative 2 calculated using s14ae: -1.6002e+04
Derivative and error estimates for derivative 2
      hbase        der(2)      erest(2)
    2.5000e-03  -1.6022e+04   5.5760e+03
    2.5000e-04  -1.6002e+04   1.2831e-07
    2.5000e-05  -1.6002e+04   6.0543e-06
    2.5000e-06  -1.6002e+04   9.5762e-04

derivative 3 calculated using s14ae:  9.6001e+05
Derivative and error estimates for derivative 3
      hbase        der(3)      erest(3)
    2.5000e-03   9.1465e+05  -7.3750e+06
    2.5000e-04   9.6001e+05   2.3718e-04
    2.5000e-05   9.6001e+05   4.2253e-02
    2.5000e-06   9.6001e+05   5.9679e+01
```