NAG Toolbox for MATLAB

c05ag

1 Purpose

c05ag locates a simple zero of a continuous function from a given starting value, using a binary search to locate an interval containing a zero of the function, then a combination of the methods of linear interpolation, extrapolation and bisection to locate the zero precisely.

2 Syntax

```
[x, a, b, ifail] = c05ag(x, h, eps, eta, f)
```

3 Description

c05ag attempts to locate an interval $[a, b]$ containing a simple zero of the function $f(x)$ by a binary search starting from the initial point $x = \mathbf{x}$ and using repeated calls to c05av. If this search succeeds, then the zero is determined to a user-specified accuracy by repeated calls to c05ad. The specifications of functions c05av and c05ad should be consulted for details of the methods used.

The approximation x to the zero α is determined so that at least one of the following criteria is satisfied:

(i) α lies within an interval $[\beta, \gamma]$ whose length satisfies $|\beta - \gamma| \leq 2 \times \mathbf{eps} \times \max(|\beta|, 1)$,

(ii) $|f(x)| < \mathbf{eta}$.

4 References

Brent R P 1973 *Algorithms for Minimization Without Derivatives* Prentice–Hall

5 Parameters

5.1 Compulsory Input Parameters

1: **x – double scalar**

An initial approximation to the zero.

2: **h – double scalar**

A step length for use in the binary search for an interval containing the zero. The maximum interval searched is $[\mathbf{x} - 256.0 \times \mathbf{h}, \mathbf{x} + 256.0 \times \mathbf{h}]$.

Constraint: **h** must be sufficiently large that $\mathbf{x} + \mathbf{h} \neq \mathbf{x}$ on the computer.

3: **eps – double scalar**

The absolute tolerance to which the zero is required (see Section 3).

Constraint: **eps** > 0.0.

4: **eta – double scalar**

A value such that if $|f(x)| \leq \mathbf{eta}$, x is accepted as the zero. **eta** may be specified as 0.0 (see Section 7).

5: **f – string containing name of m-file**

f must evaluate the function f whose zero is to be determined.

Its specification is:

```
[result] = f(xx)
```

Input Parameters

1: **xx – double scalar**

The point at which the function must be evaluated.

Output Parameters

1: **result – double scalar**

The result of the function.

5.2 Optional Input Parameters

None.

5.3 Input Parameters Omitted from the MATLAB Interface

None.

5.4 Output Parameters

1: **x – double scalar**

The final approximation to the zero, unless the function has failed, in which case it contains no useful information.

2: **a – double scalar**

3: **b – double scalar**

The lower and upper bounds respectively of the interval resulting from the binary search. If the zero is determined exactly such that $f(x) = 0.0$ or is determined so that $|f(x)| \leq$ **eta** at any stage in the calculation, then on exit $\mathbf{a} = \mathbf{b} = x$.

4: **ifail – int32 scalar**

0 unless the function detects an error (see Section 6).

6 Error Indicators and Warnings

Errors or warnings detected by the function:

ifail $= 1$

On entry, either **eps** ≤ 0.0, or $\mathbf{x} + \mathbf{h} = \mathbf{x}$ to machine accuracy (meaning that the search for an interval containing the zero cannot commence).

ifail $= 2$

An interval containing the zero could not be found. Increasing **h** and calling c05ag again will increase the range searched for the zero. Decreasing **h** and calling c05ag again will refine the mesh used in the search for the zero.

ifail $= 3$

A change of sign of $f(x)$ has been determined as occurring near the point defined by the final value of **x**. However, there is some evidence that this sign-change corresponds to a pole of $f(x)$.

ifail $= 4$

Too much accuracy has been requested in the computation; that is, the interval containing the zero has been reduced to one of relative length at most ϵ, the ***machine precision***, but the exit conditions described in Section 3 are not satisfied. It is unsafe to continue reducing the interval beyond this point, but the final value of **x** returned is an accurate approximation to the zero.

7 Accuracy

The levels of accuracy depend on the values of **eps** and **eta**. If full machine accuracy is required, they may be set very small, resulting in an exit with **ifail** $= 4$, although this may involve many more iterations than a lesser accuracy. You are recommended to set **eta** $= 0.0$ and to use **eps** to control the accuracy, unless you have considerable knowledge of the size of $f(x)$ for values of x near the zero.

8 Further Comments

The time taken by c05ag depends primarily on the time spent evaluating the function f (see Section 5). The accuracy of the initial approximation **x** and the value of **h** will have a somewhat unpredictable effect on the timing.

If it is important to determine an interval of relative length less than **eps** containing the zero, or if the user-supplied real function **f** is expensive to evaluate and the number of calls to **f** is to be restricted, then use of c05av followed by c05az is recommended. Use of this combination is also recommended when the structure of the problem to be solved does not permit a simple function f to be written: the reverse communication facilities of these functions are more flexible than the direct communication of **f** required by c05ag.

If the iteration terminates with successful exit and **a** $=$ **b** $=$ **x** there is no guarantee that the value returned in **x** corresponds to a simple zero and you should check whether it does.

One way to check this is to compute the derivative of f at the point **x**, preferably analytically, or, if this is not possible, numerically, perhaps by using a central difference estimate.

If $f'(\mathbf{x}) = 0.0$, then **x** must correspond to a multiple zero of f rather than a simple zero.

9 Example

c05ag_f.m

```
function [f] = c05agf_f(x)
  f=exp(-x)-x;
```

```
x = 1;
h = 0.1;
eps = 1e-05;
eta = 0;
[xOut, a, b, ifail] = c05ag(x, h, eps, eta, 'c05ag_f')
```

```
xOut =
    0.5671
a =
    0.5000
b =
    0.9000
ifail =
           0
```