NAG Library Function Document

nag_zero_cont_func_cntin (c05awc)

1 Purpose

nag_zero_cont_func_cntin (c05awc) attempts to locate a zero of a continuous function using a continuation method based on a secant iteration.

2 Specification

3 Description

nag_zero_cont_func_cntin (c05awc) attempts to obtain an approximation to a simple zero α of the function f(x) given an initial approximation x to α . The zero is found by a call to nag_zero_cont_func_cntin_rcomm (c05axc) whose specification should be consulted for details of the method used.

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

- (i) $|x \alpha| \sim \text{eps}$,
- (ii) |f(x)| < eta.

4 References

None.

5 Arguments

1: \mathbf{x} - double * Input/Output

On entry: an initial approximation to the zero.

On exit: if fail.code = NE_NOERROR, NE_SECANT_ITER_FAILED or NE_TOO_MANY_CALLS it contains the approximation to the zero, otherwise it contains no useful information.

2: **eps** – double *Input*

On entry: an absolute tolerance to control the accuracy to which the zero is determined. In general, the smaller the value of **eps** the more accurate **x** will be as an approximation to α . Indeed, for very small positive values of **eps**, it is likely that the final approximation will satisfy $|\mathbf{x} - \alpha| < \mathbf{eps}$. You are advised to call the function with more than one value for **eps** to check the accuracy obtained.

Constraint: eps > 0.0.

3: **eta** – double *Input*

On entry: a value such that if $|f(x)| < \mathbf{eta}$, x is accepted as the zero. \mathbf{eta} may be specified as 0.0 (see Section 7).

Mark 24 c05awc.1

c05awc NAG Library Manual

4: \mathbf{f} – function, supplied by the user

External Function

 \mathbf{f} must evaluate the function f whose zero is to be determined.

The specification of \mathbf{f} is:

double f (double x, Nag Comm *comm)

1: \mathbf{x} – double

Input

On entry: the point at which the function must be evaluated.

2: **comm** – Nag Comm *

Communication Structure

Pointer to structure of type Nag Comm; the following members are relevant to f.

```
user - double *
iuser - Integer *
p - Pointer
```

The type Pointer will be void *. Before calling nag_zero_cont_func_cntin (c05awc) you may allocate memory and initialize these pointers with various quantities for use by \mathbf{f} when called from nag_zero_cont_func_cntin (c05awc) (see Section 3.2.1.1 in the Essential Introduction).

5: **nfmax** – Integer

Input

On entry: the maximum permitted number of calls to f from nag_zero_cont_func_cntin (c05awc). If f is inexpensive to evaluate, **nfmax** should be given a large value (say > 1000).

Constraint: $\mathbf{nfmax} > 0$.

6: **comm** – Nag Comm *

Communication Structure

The NAG communication argument (see Section 3.2.1.1 in the Essential Introduction).

7: **fail** – NagError *

Input/Output

The NAG error argument (see Section 3.6 in the Essential Introduction).

6 Error Indicators and Warnings

NE BAD PARAM

On entry, argument $\langle value \rangle$ had an illegal value.

NE INT

```
On entry, \mathbf{nfmax} = \langle value \rangle. Constraint: \mathbf{nfmax} > 0.
```

NE_INTERNAL_ERROR

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please contact NAG for assistance.

A serious error occurred in an internal call to an auxiliary function.

Internal scale factor invalid for this problem. Consider using nag_zero_cont_func_cntin_rcomm (c05axc) instead and setting scal.

NE REAL

```
On entry, eps = \langle value \rangle. Constraint: eps > 0.0.
```

c05awc.2 Mark 24

NE SECANT_ITER_FAILED

Either \mathbf{f} has no zero near \mathbf{x} or too much accuracy has been requested. Check the coding of \mathbf{f} or increase \mathbf{eps} .

NE TOO MANY CALLS

More than **nfmax** calls have been made to **f**.

nfmax may be too small for the problem (because x is too far away from the zero), or f has no zero near x, or too much accuracy has been requested in calculating the zero. Increase **nfmax**, check the coding of f or increase **eps**.

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 **fail.code** = NE_SECANT_ITER_FAILED or NE_TOO_MANY_CALLS, 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 Parallelism and Performance

Not applicable.

9 Further Comments

The time taken by nag_zero_cont_func_cntin (c05awc) depends primarily on the time spent evaluating the function f (see Section 5) and on how close the initial value of \mathbf{x} is to the zero.

If a more flexible way of specifying the function f is required or if you wish to have closer control of the calculation, then the reverse communication function nag_zero_cont_func_cntin_rcomm (c05axc) is recommended instead of nag zero cont func cntin (c05awc).

10 Example

This example calculates the zero of $f(x) = e^{-x} - x$ from a starting value $\mathbf{x} = 1.0$. Two calculations are made with $\mathbf{eps} = 1.0\mathrm{e}{-3}$ and $1.0\mathrm{e}{-4}$ for comparison purposes, with $\mathbf{eta} = 0.0$ in both cases.

10.1 Program Text

```
/* nag_zero_cont_func_cntin (c05awc) Example Program.
   Copyright 2011 Numerical Algorithms Group.
 * Mark 23, 2011.
#include <nag.h>
#include <nagx04.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <math.h>
#include <nagc05.h>
#include <nagx02.h>
#ifdef __c]
extern "C"
         _cplusplus
           {
#endif
static double NAG_CALL f(double x, Nag_Comm *comm);
#ifdef __cplusplus
#endif
```

Mark 24 c05awc.3

```
int main(void)
  /* Scalars */
 Integer
                  nfmax, exit_status = 0;
 double
                   eps, eta, x, i;
 /* Arrays */
 static double ruser[1] = {-1.0};
 NagError
                   fail;
 Nag_Comm
                   comm;
 printf("nag_zero_cont_func_cntin (c05awc) Example Program Results\n");
  /* For communication with user-supplied functions: */
 comm.user = ruser;
 for (i = 3; i \le 4; i++)
     eps = pow(10.0, -i);
      x = 1.0;
     eta = 0.0;
     nfmax = 200;
     INIT_FAIL(fail);
      /* nag_zero_cont_func_cntin (c05awc).
      * Locates a zero of a continuous function.
     nag_zero_cont_func_cntin(&x, eps, eta, f, nfmax, &comm, &fail);
      if (fail.code == NE_NOERROR)
         printf("\nWith eps = 10.2e, root is 14.5f\n", eps, x);
        }
      else
        {
          printf(
                  "Error from nag_zero_cont_func_cntin (c05awc) s\n'',
                  fail.message);
          if (fail.code == NE_TOO_MANY_CALLS ||
              fail.code == NE_SECANT_ITER_FAILED)
              printf("\nWith eps = %10.2e, final value is %14.5f\n",
                      eps, x);
            }
          exit_status = 1;
          goto END;
    }
END:
 return exit_status;
}
static double NAG_CALL f(double x, Nag_Comm *comm)
  if (comm->user[0] == -1.0)
     printf("(User-supplied callback f, first invocation.)\n");
     comm->user[0] = 0.0;
 return exp(-x)-x;
```

10.2 Program Data

None.

c05awc.4 Mark 24

10.3 Program Results

nag_zero_cont_func_cntin (c05awc) Example Program Results
(User-supplied callback f, first invocation.)

With eps = 1.00e-03, root is 0.56715With eps = 1.00e-04, root is 0.56715

Mark 24 c05awc.5 (last)