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

#include <nag.h>
#include <nagc05.h>

void nag_zero_cont_func_cntin (double *x, double eps, double eta,
   double (*f)(double x, Nag_Comm *comm),
   Integer nfmax, Nag_Comm *comm, NagError *fail)

3 Description

nag_zero_cont_func_cntin (c05awc) attempts to obtain an approximation to a simple zero $\alpha$ of the
function $f(x)$ given an initial approximation $x$ to $\alpha$. 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 $\alpha$ is determined so that at least one of the following criteria is satisfied:

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

4 References

None.

5 Arguments

1: $x$ – double *
   $x$ – an initial approximation to the zero.
   *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: $\text{eps}$ – double
   $\text{eps}$ – an absolute tolerance to control the accuracy to which the zero is determined. In general,
   the smaller the value of $\text{eps}$ the more accurate $x$ will be as an approximation to $\alpha$. Indeed, for very
   small positive values of $\text{eps}$, it is likely that the final approximation will satisfy $|x - \alpha| < \text{eps}$. You
   are advised to call the function with more than one value for $\text{eps}$ to check the accuracy obtained.
   *Input*
   On entry: an absolute tolerance to control the accuracy to which the zero is determined. In general,
   the smaller the value of $\text{eps}$ the more accurate $x$ will be as an approximation to $\alpha$. Indeed, for very
   small positive values of $\text{eps}$, it is likely that the final approximation will satisfy $|x - \alpha| < \text{eps}$. You
   are advised to call the function with more than one value for $\text{eps}$ to check the accuracy obtained.
   *Constraint*: $\text{eps} > 0.0$.

3: $\text{eta}$ – double
   $\text{eta}$ – a value such that if $|f(x)| < \text{eta}$, $x$ is accepted as the zero. $\text{eta}$ may be specified as 0.0
   (see Section 7).
   *Input*
4: \( f \) – function, supplied by the user

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

The specification of \( f \) is:

```c
double f (double x, Nag_Comm *comm)
```

1: \( x \) – double

*Input*

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

2: \( \text{comm} \) – Nag_Comm *

Pointer to structure of type Nag_Comm; the following members are relevant to \( f \).

\[\begin{align*}
\text{user} & \quad \text{double *} \\
\text{iuser} & \quad \text{Integer *} \\
\text{p} & \quad \text{Pointer}
\end{align*}\]

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

5: \( \text{nfmax} \) – Integer

*Input*

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

Constraint: \( \text{nfmax} > 0 \).

6: \( \text{comm} \) – Nag_Comm *

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

7: \( \text{fail} \) – NagError *

*Input/Output*

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

6 \ Error Indicators and Warnings

**NE_ALLOC_FAIL**

Dynamic memory allocation failed.

See Section 3.2.1.2 in the Essential Introduction for further information.

**NE_BAD_PARAM**

On entry: argument \( \langle \text{value} \rangle \) had an illegal value.

**NE_INT**

On entry, \( \text{nfmax} = \langle \text{value} \rangle \).

Constraint: \( \text{nfmax} > 0 \).

**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.

An unexpected error has been triggered by this function. Please contact NAG.

See Section 3.6.6 in the Essential Introduction for further information.

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_NO_LICENCE**

Your licence key may have expired or may not have been installed correctly. See Section 3.6.5 in the Essential Introduction for further information.

**NE_REAL**

On entry, eps = (value).
Constraint: eps > 0.0.

**NE_SECANT_ITER_FAILED**

Either f has no zero near x or too much accuracy has been requested. Check the coding of f or increase 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 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 x = 1.0. Two calculations are made with eps = 1.0e−3 and 1.0e−4 for comparison purposes, with eta = 0.0 in both cases.

10.1 Program Text

/* nag_zero_cont_func_cntin (c05awc) Example Program. *
 * Copyright 2014 Numerical Algorithms Group. *
 * Mark 23, 2011. */

#include <nag.h>

Mark 25
```c
#include <nagx04.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <math.h>
#include <nagc05.h>
#include <nagx02.h>

#ifdef __cplusplus
extern "C" {
#endif
static double NAG_CALL f(double x, Nag_Comm *comm);
#ifdef __cplusplus
}
#endif

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 <= 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("With 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("With 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.

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