NAG Library Function Document

nag_opt_one_var_deriv (e04bbc)

1 Purpose

nag_opt_one_var_deriv (e04bbc) searches for a minimum, in a given finite interval, of a continuous function of a single variable, using function and first derivative values. The method (based on cubic interpolation) is intended for functions which have a continuous first derivative (although it will usually work if the derivative has occasional discontinuities).

2 Specification

```
#include <nag.h>
#include <nage04.h>
```

```
void nag_opt_one_var_deriv (void (*funct)(double xc, double *fc, double *gc,
     Nag_Comm *comm),
     double e1, double e2, double *a, double *b, Integer max_fun, double *x,
     double *f, double *g, Nag_Comm *comm, NagError *fail)
```

3 Description

nag_opt_one_var_deriv (e04bbc) is applicable to problems of the form:

$$\text{Minimize} \quad F(x) \quad \text{subject to} \quad a \leq x \leq b$$

when the first derivative dF/dx can be calculated. nag_opt_one_var_deriv (e04bbc) normally computes a sequence of x values which tend in the limit to a minimum of $F(x)$ subject to the given bounds. It also progressively reduces the interval $[a, b]$ in which the minimum is known to lie. It uses the safeguarded quadratic-interpolation method described in Gill and Murray (1973).

You must supply a function **funct** to evaluate $F(x)$ and its first derivative. The arguments **e1** and **e2** together specify the accuracy:

$$Tol(x) = \mathbf{e1} \times |x| + \mathbf{e2}$$

to which the position of the minimum is required. Note that **funct** is never called at any point which is closer than $Tol(x)$ to a previous point.

If the original interval $[a, b]$ contains more than one minimum,nag_opt_one_var_deriv (e04bbc) will normally find one of the minima.

4 References

Gill P E and Murray W (1973) Safeguarded steplength algorithms for optimization using descent methods *NPL Report NAC 37* National Physical Laboratory

5 Arguments

1: **funct** – function, supplied by the user *External Function*

funct must calculate the values of $F(x)$ and dF/dx at any point x in $[a, b]$.

The specification of **funct** is:

```
void funct (double xc, double *fc, double *gc, Nag_Comm *comm)
```

1: **xc** – double *Input*

On entry: x, the point at which the values of F and dF/dx are required.

2: **fc** – double * *Output*

On exit: the value of the function F at the current point x.

3: **gc** – double * *Output*

On exit: the value of the first derivative dF/dx at the current point x.

4: **comm** – Nag_Comm *

Pointer to structure of type Nag_Comm; the following members are relevant to **funct**.

first – Nag_Boolean *Input*

On entry: will be set to Nag_TRUE on the first call to **funct** and Nag_FALSE for all subsequent calls.

nf – Integer *Input*

On entry: the number of calls made to **funct** so far.

user – double *
iuser – Integer *
p – Pointer

The type Pointer will be `void *` with a C compiler that defines `void *` and `char *` otherwise. Before calling nag_opt_one_var_deriv (e04bbc) these pointers may be allocated memory and initialized with various quantities for use by **funct** when called from nag_opt_one_var_deriv (e04bbc).

Note: **funct** should be tested separately before being used in conjunction with nag_opt_one_var_deriv (e04bbc).

2: **e1** – double *Input*

On entry: the relative accuracy to which the position of a minimum is required. (Note that since **e1** is a relative tolerance, the scaling of x is automatically taken into account.)

It is recommended that **e1** should be no smaller than 2ϵ, and preferably not much less than $\sqrt{\epsilon}$, where ϵ is the ***machine precision***.

If **e1** is set to a value less than ϵ, its value is ignored and the default value of $\sqrt{\epsilon}$ is used instead. In particular, you may set **e1** $= 0.0$ to ensure that the default value is used.

3: **e2** – double *Input*

On entry: the absolute accuracy to which the position of a minimum is required. It is recommended that **e2** should be no smaller than 2ϵ.

If **e2** is set to a value less than ϵ, its value is ignored and the default value of $\sqrt{\epsilon}$ is used instead. In particular, you may set **e2** $= 0.0$ to ensure that the default value is used.

4: **a** – double * *Input/Output*

On entry: the lower bound a of the interval containing a minimum.

On exit: an improved lower bound on the position of the minimum.

5: **b** – double * *Input/Output*

On entry: the upper bound b of the interval containing a minimum.

On exit: an improved upper bound on the position of the minimum.

Constraint: $\mathbf{b} > \mathbf{a} + \mathbf{e2}$.

Note that the value $\mathbf{e2} = \sqrt{\epsilon}$ applies here if $\mathbf{e2} < \epsilon$ on entry to nag_opt_one_var_deriv (e04bbc).

6: **max_fun** – Integer *Input*

On entry: the maximum number of calls to **funct** which you are prepared to allow.

The number of calls to **funct** actually made by nag_opt_one_var_deriv (e04bbc) may be determined by supplying a non-NULL argument **comm** (see below) and examining the structure member **comm** → **nf** on exit.

Constraint: **max_fun** ≥ 2.

(Few problems will require more than 20 function calls.)

7: **x** – double * *Output*

On exit: the estimated position of the minimum.

8: **f** – double * *Output*

On exit: the value of F at the final point **x**.

9: **g** – double * *Output*

On exit: the value of the first derivative dF/dx at the final point **x**.

10: **comm** – Nag_Comm * *Input/Output*

Note: **comm** is a NAG defined type (see Section 3.2.1.1 in the Essential Introduction).

On entry/exit: structure containing pointers for communication to user-supplied functions; see the above description of **funct** for details. The number of times the function **funct** was called is returned in the member **comm** → **nf**.

If you do not need to make use of this communication feature, the null pointer `NAGCOMM_NULL` may be used in the call to nag_opt_one_var_deriv (e04bbc); **comm** will then be declared internally for use in calls to user-supplied functions.

11: **fail** – NagError * *Input/Output*

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

6 Error Indicators and Warnings

NE_2_REAL_ARG_GE

On entry, $\mathbf{a} + \mathbf{e2} = \langle value \rangle$ while $\mathbf{b} = \langle value \rangle$. These arguments must satisfy $\mathbf{a} + \mathbf{e2} < \mathbf{b}$.

NE_INT_ARG_LT

On entry, **max_fun** must not be less than 2: **max_fun** $= \langle value \rangle$.

NW_MAX_FUN

The maximum number of function calls, $\langle value \rangle$, have been performed.

This may have happened simply because **max_fun** was set too small for a particular problem, or may be due to a mistake in the user-supplied function, **funct**. If no mistake can be found in **funct**, restart nag_opt_one_var_deriv (e04bbc) (preferably with the values of **a** and **b** given on exit from the previous call to nag_opt_one_var_deriv (e04bbc)).

7 Accuracy

If $F(x)$ is δ-unimodal for some $\delta < Tol(x)$, where $Tol(x) = \mathbf{e1} \times |x| + \mathbf{e2}$, then, on exit, x approximates the minimum of $F(x)$ in the original interval $[a, b]$ with an error less than $3 \times Tol(x)$.

8 Further Comments

Timing depends on the behaviour of $F(x)$, the accuracy demanded, and the length of the interval $[a, b]$. Unless $F(x)$ and dF/dx can be evaluated very quickly, the run time will usually be dominated by the time spent in **funct**.

If $F(x)$ has more than one minimum in the original interval $[a, b]$, nag_opt_one_var_deriv (e04bbc) will determine an approximation x (and improved bounds a and b) for one of the minima.

If nag_opt_one_var_deriv (e04bbc) finds an x such that $F(x - \delta_1) > F(x) < F(x + \delta_2)$ for some $\delta_1, \delta_2 \geq Tol(x)$, the interval $[x - \delta_1, x + \delta_2]$ will be regarded as containing a minimum, even if $F(x)$ is less than $F(x - \delta_1)$ and $F(x + \delta_2)$ only due to rounding errors in the user-supplied function. Therefore **funct** should be programmed to calculate $F(x)$ as accurately as possible, so that nag_opt_one_var_deriv (e04bbc) will not be liable to find a spurious minimum. (For similar reasons, dF/dx should be evaluated as accurately as possible.)

9 Example

A sketch of the function

$$F(x) = \frac{\sin x}{x}$$

shows that it has a minimum somewhere in the range $[3.5, 5.0]$. The example program below shows how nag_opt_one_var_deriv (e04bbc) can be used to obtain a good approximation to the position of a minimum.

9.1 Program Text

```
/* nag_opt_one_var_deriv (e04bbc) Example Program.
 *
 * Copyright 1998 Numerical Algorithms Group.
 *
 * Mark 5, 1998.
 * Mark 7 revised, 2001.
 * Mark 8 revised, 2004.
 *
 */

#include <nag.h>
#include <nagx04.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <math.h>
#include <nage04.h>

#ifdef __cplusplus
extern "C" {
#endif
static void NAG_CALL funct(double xc, double *fc, double *gc, Nag_Comm *comm);
#ifdef __cplusplus
}
#endif

static void NAG_CALL funct(double xc, double *fc, double *gc, Nag_Comm *comm)
{
  *fc = sin(xc) / xc;
  *gc = (cos(xc) - *fc) / xc;
}
/* funct */
```

```
int main(int argc, char *argv[])
{
  FILE     *fpout;
  Integer  exit_status = 0, max_fun;
  NagError fail;
  Nag_Comm comm;
  double   a, b, e1, e2, f, g, x;

  INIT_FAIL(fail);

  /* Check for command-line IO options */
  fpout = nag_example_file_io(argc, argv, "-results", NULL);

  fprintf(fpout, "nag_opt_one_var_deriv (e04bbc) Example Program Results\n\n");

  /* e1 and e2 are set to zero so that nag_opt_one_var_no_deriv (e04abc) will
   *  reset them to their default values
   */
  e1 = 0.0;
  e2 = 0.0;
  /* The minimum is known to lie in the range (3.5, 5.0) */
  a = 3.5;
  b = 5.0;
  /* Allow 30 calls of funct */
  max_fun = 30;
  /* nag_opt_one_var_deriv (e04bbc).
   * Minimizes a function of one variable, requires first
   * derivatives
   */
  nag_opt_one_var_deriv(funct, e1, e2, &a, &b, max_fun, &x, &f, &g, &comm,
                        &fail);
  if (fail.code != NE_NOERROR)
    {
      fprintf(fpout, "Error from nag_opt_one_var_deriv (e04bbc).\n%s\n",
              fail.message);
      exit_status = 1;
      goto END;
    }

  fprintf(fpout, "The minimum lies in the interval %7.5f to %7.5f.\n", a, b);
  fprintf(fpout, "Its estimated position is %7.5f,\n", x);
  fprintf(fpout, "where the function value is %13.4e\n", f);
  fprintf(fpout, "and the gradient is %13.4e.\n", g);
  fprintf(fpout, "%1ld function evaluations were required.\n", comm.nf);
 END:
  if (fpout != stdout) fclose(fpout);
  return exit_status;
}
```

9.2 Program Data

None.

9.3 Program Results

```
nag_opt_one_var_deriv (e04bbc) Example Program Results

The minimum lies in the interval 4.49341 to 4.49341.
Its estimated position is 4.49341,
where the function value is   -2.1723e-01
and the gradient is   -3.7679e-16.
6 function evaluations were required.
```
