NAG Library Function Document

nag_opt_bounds_deriv (e04kbc)

1 Purpose

nag_opt_bounds_deriv (e04kbc) is a comprehensive quasi-Newton algorithm for finding:

– an unconstrained minimum of a function of several variables;

– a minimum of a function of several variables subject to fixed upper and/or lower bounds on the variables.

First derivatives are required. nag_opt_bounds_deriv (e04kbc) is intended for objective functions which have continuous first and second derivatives (although it will usually work even if the derivatives have occasional discontinuities).

2 Specification

```
#include <nag.h>
#include <nage04.h>
void nag_opt_bounds_deriv (Integer n,
     void (*objfun)(Integer n, const double x[], double *objf, double g[],
          Nag_Comm *comm),
     Nag_BoundType bound, double bl[], double bu[], double x[], double *objf,
     double g[], Nag_E04_Opt *options, Nag_Comm *comm, NagError *fail)
```

3 Description

nag_opt_bounds_deriv (e04kbc) is applicable to problems of the form:

$$\begin{array}{ll} \text{Minimize} & F(x_1, x_2, \ldots, x_n) \\ \text{subject to} & l_j \leq x_j \leq u_j, \quad j = 1, 2, \ldots, n. \end{array}$$

Special provision is made for unconstrained minimization (i.e., problems which actually have no bounds on the x_j), problems which have only non-negativity bounds, and problems in which $l_1 = l_2 = \cdots = l_n$ and $u_1 = u_2 = \cdots = u_n$. It is possible to specify that a particular x_j should be held constant. You must supply a starting point and a function **objfun** to calculate the value of $F(x)$ and its first derivatives $\frac{\partial F}{\partial x_j}$ at any point x.

A typical iteration starts at the current point x where n_z (say) variables are free from both their bounds. The vector g_z, whose elements are the derivatives of $F(x)$ with respect to the free variables, is known. A unit lower triangular matrix L and a diagonal matrix D (both of dimension n_z), such that LDL^{T} is a positive definite approximation to the matrix of second derivatives with respect to the free variables, are also stored. The equations

$$LDL^{\mathrm{T}} p_z = -g_z$$

are solved to give a search direction p_z, which is expanded to an n-vector p by the insertion of appropriate zero elements. Then α is found such that $F(x + \alpha p)$ is approximately a minimum (subject to the fixed bounds) with respect to α; x is replaced by $x + \alpha p$, and the matrices L and D are updated so as to be consistent with the change produced in the gradient by the step αp. If any variable actually reaches a bound during the search along p, it is fixed and n_z is reduced for the next iteration.

There are two sets of convergence criteria – a weaker and a stronger. Whenever the weaker criteria are satisfied, the Lagrange-multipliers are estimated for all the active constraints. If any Lagrange-multiplier estimate is significantly negative, then one of the variables associated with a negative Lagrange-multiplier estimate is released from its bound and the next search direction is computed in the extended subspace (i.e., n_z is increased). Otherwise minimization continues in the current subspace provided that this is practicable. When it is not, or when the stronger convergence criteria is already satisfied, then, if one or more Lagrange-multiplier estimates are close to zero, a slight perturbation is made in the values of the corresponding variables in turn until a lower function value is obtained. The normal algorithm is then resumed from the perturbed point.

If a saddle point is suspected, a local search is carried out with a view to moving away from the saddle point. In addition, nag_opt_bounds_deriv (e04kbc) gives you the option of specifying that a local search should be performed when a point is found which is thought to be a constrained minimum.

If you specify that the problem is unconstrained, nag_opt_bounds_deriv (e04kbc) sets the l_j to -10^{10} and the u_j to 10^{10}. Thus, provided that the problem has been sensibly scaled, no bounds will be encountered during the minimization process and nag_opt_bounds_deriv (e04kbc) will act as an unconstrained minimization algorithm.

4 References

Gill P E and Murray W (1972) Quasi-Newton methods for unconstrained optimization *J. Inst. Math. Appl.* **9** 91–108

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

Gill P E and Murray W (1976) Minimization subject to bounds on the variables *NPL Report NAC 72* National Physical Laboratory

Gill P E, Murray W and Pitfield R A (1972) The implementation of two revised quasi-Newton algorithms for unconstrained optimization *NPL Report NAC 11* National Physical Laboratory

5 Arguments

1: **n** – Integer *Input*

On entry: the number n of independent variables.

Constraint: **n** ≥ 1.

2: **objfun** – function, supplied by the user *External Function*

objfun must evaluate the function $F(x)$ and its first derivatives $\dfrac{\partial F}{\partial x_j}$ at any point x. (However, if you do not wish to calculate $F(x)$ or its first derivatives at a particular x, there is the option of setting an argument to cause nag_opt_bounds_deriv (e04kbc) to terminate immediately.)

The specification of **objfun** is:

```
void objfun (Integer n, const double x[], double *objf, double g[],
     Nag_Comm *comm)
```

1: **n** – Integer *Input*

On entry: the number n of variables.

2: **x**[**n**] – const double *Input*

On entry: the point x at which the value of F, or F and $\dfrac{\partial F}{\partial x_j}$, are required.

3: **objf** – double * *Output*

On exit: **objfun** must set **objf** to the value of the objective function F at the current point x. If it is not possible to evaluate F, then **objfun** should assign a negative value to **comm→flag**; nag_opt_bounds_deriv (e04kbc) will then terminate.

4: **g**[**n**] – double *Output*

On exit: if **comm**→**flag** $= 2$ on entry, then **objfun** must set **g**$[j-1]$ to the value of the first derivative $\frac{\partial F}{\partial x_j}$ at the current point, x for $j = 1, 2, \ldots, n$. If it is not possible to evaluate the first derivatives then **objfun** should assign a negative value to **comm**→**flag**; nag_opt_bounds_deriv (e04kbc) will then terminate.

(If **comm**→**flag** $= 0$ on entry, **objfun** must **not** change the elements of **g**.)

5: **comm** – Nag_Comm *

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

flag – Integer *Input/Output*

On entry: **comm**→**flag** will be set to 0 or 2. The value 0 indicates that only F itself needs to be evaluated. The value 2 indicates that both F and its first derivatives must be calculated.

On exit: if **objfun** resets **comm**→**flag** to some negative number then nag_opt_bounds_deriv (e04kbc) will terminate immediately with the error indicator NE_USER_STOP. If **fail** is supplied to nag_opt_bounds_deriv (e04kbc), **fail**.**errnum** will be set to your setting of **comm**→**flag**.

first – Nag_Boolean *Input*

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

nf – Integer *Input*

On entry: the number of calculations of the objective function; this value will be equal to the number of calls made to **objfun**, including the current one.

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_bounds_deriv (e04kbc) these pointers may be allocated memory and initialized with various quantities for use by **objfun** when called from nag_opt_bounds_deriv (e04kbc).

Note: **objfun** should be tested separately before being used in conjunction with nag_opt_bounds_deriv (e04kbc). The array **x** must **not** be changed by **objfun**.

3: **bound** – Nag_BoundType *Input*

On entry: indicates whether the problem is unconstrained or bounded and, if it is bounded, whether the facility for dealing with bounds of special forms is to be used. **bound** should be set to one of the following values:

bound = Nag_Bounds
If the variables are bounded and you will be supplying all the l_j and u_j individually.

bound = Nag_NoBounds
If the problem is unconstrained.

bound = Nag_BoundsZero
If the variables are bounded, but all the bounds are of the form $0 \leq x_j$.

bound = Nag_BoundsEqual
If all the variables are bounded, and $l_1 = l_2 = \cdots = l_n$ and $u_1 = u_2 = \cdots = u_n$.

Constraint: **bound** = Nag_Bounds, Nag_NoBounds, Nag_BoundsZero or Nag_BoundsEqual.

4: **bl**[**n**] – double *Input/Output*

On entry: the lower bounds l_j.

If **bound** = Nag_Bounds, you must set **bl**$[j-1]$ to l_j, for $j = 1, 2, \ldots, n$. (If a lower bound is not required for any x_j, the corresponding **bl**$[j-1]$ should be set to a large negative number, e.g., -10^{10}.)

If **bound** = Nag_BoundsEqual, you must set **bl**[0] to l_1; nag_opt_bounds_deriv (e04kbc) will then set the remaining elements of **bl** equal to **bl**[0].

If **bound** = Nag_NoBounds or Nag_BoundsZero, **bl** will be initialized by nag_opt_bounds_deriv (e04kbc).

On exit: the lower bounds actually used by nag_opt_bounds_deriv (e04kbc), e.g., if **bound** = Nag_BoundsZero, **bl**[0] = **bl**[1] = $\cdots$ = **bl**$[n-1]$ = 0.0.

5: **bu**[**n**] – double *Input/Output*

On entry: the upper bounds u_j.

If **bound** = Nag_Bounds, you must set **bu**$[j-1]$ to u_j, for $j = 1, 2, \ldots, n$. (If an upper bound is not required for any x_j, the corresponding **bu**$[j-1]$ should be set to a large positive number, e.g., 10^{10}.)

If **bound** = Nag_BoundsEqual, you must set **bu**[0] to u_1; nag_opt_bounds_deriv (e04kbc) will then set the remaining elements of **bu** equal to **bu**[0].

If **bound** = Nag_NoBounds or Nag_BoundsZero, **bu** will be initialized by nag_opt_bounds_deriv (e04kbc).

On exit: the upper bounds actually used by nag_opt_bounds_deriv (e04kbc), e.g., if **bound** = Nag_BoundsZero, **bu**[0] = **bu**[1] = $\cdots$ = **bu**$[n-1]$ = 10^{10}.

6: **x**[**n**] – double *Input/Output*

On entry: **x**$[j-1]$ must be set to a guess at the jth component of the position of the minimum, for $j = 1, 2, \ldots, n$.

On exit: the final point x^*. Thus, if **fail.code** = NE_NOERROR on exit, **x**$[j-1]$ is the jth component of the estimated position of the minimum.

7: **objf** – double * *Input/Output*

On entry: if **options.init_state** = Nag_Init_None or Nag_Init_H_S, you need not initialize **objf**.

If **options.init_state** = Nag_Init_F_G_H or Nag_Init_All, **objf** must be set on entry to the value of $F(x)$ at the initial point supplied in **x**.

On exit: the function value at the final point given in **x**.

8: **g**[**n**] – double *Input/Output*

On entry:

options.init_state = Nag_Init_F_G_H or Nag_Init_All
g must be set on entry to the first derivative vector at the initial x.

options.init_state = Nag_Init_None or Nag_Init_H_S
g need not be set.

On exit: the first derivative vector corresponding to the final point in **x**. The elements of **g** corresponding to free variables should normally be close to zero.

9: **options** – Nag_E04_Opt * *Input/Output*

On entry/exit: a pointer to a structure of type Nag_E04_Opt whose members are optional arguments for nag_opt_bounds_deriv (e04kbc). These structure members offer the means of adjusting some of the argument values of the algorithm and on output will supply further details of the results. A description of the members of **options** is given below in Section 11. Some of the results returned in **options** can be used by nag_opt_bounds_deriv (e04kbc) to perform a 'warm start' if it is re-entered (see the member **options.init_state** in Section 11.2).

If any of these optional arguments are required then the structure **options** should be declared and initialized by a call to nag_opt_init (e04xxc) and supplied as an argument to nag_opt_bounds_deriv (e04kbc). However, if the optional arguments are not required the NAG defined null pointer, `E04_DEFAULT`, can be used in the function call.

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 with user-supplied functions; see the above description of **objfun** for details. 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_bounds_deriv (e04kbc); **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).

5.1 Description of Printed Output

Intermediate and final results are printed out by default. The level of printed output can be controlled with the structure member **options.print_level** (see Section 11.2). The default, **options.print_level** = Nag_Soln_Iter, provides a single line of output at each iteration and the final result. This section describes the default printout produced by nag_opt_bounds_deriv (e04kbc).

The following line of output is produced at each iteration. In all cases the values of the quantities printed are those in effect *on completion* of the given iteration.

`Itn` the iteration count, k.

`Nfun` the cumulative number of calls made to **objfun**.

`Objective` the value of the objective function, $F\left(x^{(k)}\right)$

`Norm g` the Euclidean norm of the projected gradient vector, $\left\|g_z\left(x^{(k)}\right)\right\|$.

`Norm x` the Euclidean norm of $x^{(k)}$.

`Norm(x(k-1)-x(k))` the Euclidean norm of $x^{(k-1)} - x^{(k)}$.

`Step` the step $\alpha^{(k)}$ taken along the computed search direction $p^{(k)}$.

`Cond H` the ratio of the largest to the smallest element of the diagonal factor D of the projected Hessian matrix. This quantity is usually a good estimate of the condition number of the projected Hessian matrix. (If no variables are currently free, this value will be zero.)

The printout of the final result consists of:

`x` the final point, x^*.

`g` the final projected gradient vector, $g_z(x^*)$.

`Status` the final state of the variable with respect to its bound(s).

6 Error Indicators and Warnings

When one of NE_USER_STOP, NE_INT_ARG_LT, NE_BOUND, NE_DERIV_ERRORS, NE_OPT_-NOT_INIT, NE_BAD_PARAM, NE_2_REAL_ARG_LT, NE_INVALID_INT_RANGE_1, NE_INVALI-D_REAL_RANGE_EF, NE_INVALID_REAL_RANGE_FF, NE_INIT_MEM, NE_NO_MEM, NE_HESD or NE_ALLOC_FAIL occurs, no values will have been assigned by nag_opt_bounds_deriv (e04kbc) to **objf** or to the elements of **g**, **options**.**hesl**, or **options**.**hesd**.

An exit of **fail**.**code** = NW_TOO_MANY_ITER, NW_COND_MIN and NW_LOCAL_SEARCH may also be caused by mistakes in **objfun**, by the formulation of the problem or by an awkward function. If there are no such mistakes, it is worth restarting the calculations from a different starting point (not the point at which the failure occurred) in order to avoid the region which caused the failure.

NE_2_REAL_ARG_LT

On entry, **options**.**step_max** = ⟨*value*⟩ while **options**.**optim_tol** = ⟨*value*⟩. These arguments must satisfy **options**.**step_max** $\geq$ **options**.**optim_tol**.

NE_ALLOC_FAIL

Dynamic memory allocation failed.

NE_BAD_PARAM

On entry, argument **bound** had an illegal value.

On entry, argument **options**.**init_state** had an illegal value.

On entry, argument **options**.**print_level** had an illegal value.

NE_BOUND

The lower bound for variable ⟨*value*⟩ (array element **bl**[⟨*value*⟩]) is greater than the upper bound.

NE_CHOLESKY_OVERFLOW

An overflow would have occurred during the updating of the Cholesky factors if the calculations had been allowed to continue. Restart from the current point with
options.**init_state** = Nag_Init_None.

NE_DERIV_ERRORS

Large errors were found in the derivatives of the objective function.

NE_HESD

The initial values of the supplied **options**.**hesd** has some value(s) which is negative or too small or the ratio of the largest element of **options**.**hesd** to the smallest is too large.

NE_INIT_MEM

Option **options**.**init_state** = ⟨*string*⟩ but the pointer ⟨*string*⟩ in the option structure has not been allocated memory.

NE_INT_ARG_LT

On entry, **n** = ⟨*value*⟩.
Constraint: **n** ≥ 1.

NE_INVALID_INT_RANGE_1

Value ⟨*value*⟩ given to **options**.**max_iter** is not valid. Correct range is **options**.**max_iter** ≥ 0.

NE_INVALID_REAL_RANGE_EF

Value ⟨*value*⟩ given to **options**.**optim_tol** not valid. Correct range is $\epsilon \leq$ **options**.**optim_tol** < 1.0.

NE_INVALID_REAL_RANGE_FF

Value ⟨*value*⟩ given to **options.linesearch_tol** not valid. Correct range is $0.0 \leq$ **options.linesearch_tol** < 1.0.

NE_NO_MEM

Option **options.init_state** $= \langle string \rangle$ but at least one of the pointers $\langle string \rangle$ in the option structure has not been allocated memory.

NE_NOT_APPEND_FILE

Cannot open file $\langle string \rangle$ for appending.

NE_NOT_CLOSE_FILE

Cannot close file $\langle string \rangle$.

NE_OPT_NOT_INIT

Options structure not initialized.

NE_USER_STOP

User requested termination, user flag value $= \langle$*value*$\rangle$.

This exit occurs if you set **comm→flag** to a negative value in **objfun**. If **fail** is supplied the value of **fail.errnum** will be the same as your setting of **comm→flag**.

NE_WRITE_ERROR

Error occurred when writing to file $\langle string \rangle$.

NW_COND_MIN

The conditions for a minimum have not all been satisfied, but a lower point could not be found.

Provided that, on exit, the first derivatives of $F(x)$ with respect to the free variables are sufficiently small, and that the estimated condition number of the second derivative matrix is not too large, this error exit may simply mean that, although it has not been possible to satisfy the specified requirements, the algorithm has in fact found the minimum as far as the accuracy of the machine permits. This could be because **options.optim_tol** has been set so small that rounding error in **objfun** makes attainment of the convergence conditions impossible.

If the estimated condition number of the approximate Hessian matrix at the final point is large, it could be that the final point is a minimum but that the smallest eigenvalue of the second derivative matrix is so close to zero that it is not possible to recognize the point as a minimum.

NW_LOCAL_SEARCH

The local search has failed to find a feasible point which gives a significant change of function value.

If the problem is a genuinely unconstrained one, this type of exit indicates that the problem is extremely ill conditioned or that the function has no minimum. If the problem has bounds which may be close to the minimum, it may just indicate that steps in the subspace of free variables happened to meet a bound before they changed the function value.

NW_TOO_MANY_ITER

The maximum number of iterations, ⟨*value*⟩, have been performed.

If steady reductions in $F(x)$, were monitored up to the point where this exit occurred, then the exit probably occurred simply because **options.max_iter** was set too small, so the calculations should be restarted from the final point held in **x**. This exit may also indicate that $F(x)$ has no minimum.

7 Accuracy

A successful exit (**fail**.**code** $=$ NE_NOERROR) is made from nag_opt_bounds_deriv (e04kbc) when (B1, B2 and B3) or B4 hold, and the local search (if used) confirms a minimum, where

$$\text{B1} \equiv \alpha^{(k)} \times \left\|p^{(k)}\right\| < (\textbf{options.optim\_tol} + \sqrt{\epsilon}) \times \left(1.0 + \left\|x^{(k)}\right\|\right)$$

$$\text{B2} \equiv \left|F^{(k)} - F^{(k-1)}\right| < \left(\textbf{options.optim\_tol}^2 + \epsilon\right) \times \left(1.0 + \left|F^{(k)}\right|\right)$$

$$\text{B3} \equiv \left\|g_z^{(k)}\right\| < \left(\epsilon^{1/3} + \textbf{options.optim\_tol}\right) \times \left(1.0 + \left|F^{(k)}\right|\right)$$

$$\text{B4} \equiv \left\|g_z^{(k)}\right\| < 0.01 \times \sqrt{\epsilon}.$$

(Quantities with superscript k are the values at the kth iteration of the quantities mentioned in Section 3; ϵ is the ***machine precision***, $\|.\|$ denotes the Euclidean norm and **options**.**optim_tol** is described in Section 11.)

If **fail**.**code** $=$ NE_NOERROR, then the vector in **x** on exit, x_{sol}, is almost certainly an estimate of the position of the minimum, x_{true}, to the accuracy specified by **options**.**optim_tol**.

If **fail**.**code** $=$ NW_COND_MIN or NW_LOCAL_SEARCH, x_{sol} may still be a good estimate of x_{true}, but the following checks should be made. Let the largest of the first n_z elements of **options**.**hesd** be **options**.**hesd**$[b]$, let the smallest be **options**.**hesd**$[s]$, and define $k =$ **options**.**hesd**$[b]$/**options**.**hesd**$[s]$. The scalar k is usually a good estimate of the condition number of the projected Hessian matrix at x_{sol}. If

(a) the sequence $\left\{F\left(x^{(k)}\right)\right\}$ converges to $F(x_{\text{sol}})$ at a superlinear or a fast linear rate,

(b) $\|g_z(x_{\text{sol}})\|^2 < 10.0 \times \epsilon$, and

(c) $k < 1.0/\|g_z(x_{\text{sol}})\|$,

then it is almost certain that x_{sol} is a close approximation to the position of a minimum. When (b) is true, then usually $F(x_{\text{sol}})$ is a close approximation to $F(x_{\text{true}})$. The quantities needed for these checks are all available in the results printout from nag_opt_bounds_deriv (e04kbc); in particular the final value of `Cond H` gives k.

Further suggestions about confirmation of a computed solution are given in the e04 Chapter Introduction.

8 Parallelism and Performance

Not applicable.

9 Further Comments

9.1 Timing

The number of iterations required depends on the number of variables, the behaviour of $F(x)$, the accuracy demanded and the distance of the starting point from the solution. The number of multiplications performed in an iteration of nag_opt_bounds_deriv (e04kbc) is roughly proportional to n_z^2. In addition, each iteration makes at least one call of **objfun** with **comm**$\rightarrow$**flag** $= 2$ if **options**.**minlin** $=$ Nag_Lin_Deriv is used or one call of **objfun** with **comm**$\rightarrow$**flag** $= 0$ if **options**.**minlin** $=$ Nag_Lin_NoDeriv is chosen. So, unless $F(x)$ can be evaluated very quickly, the run time will be dominated by the time spent in **objfun**.

9.2 Scaling

Ideally, the problem should be scaled so that, at the solution, $F(x)$ and the corresponding values of the x_j are each in the range $(-1, +1)$, and so that at points one unit away from the solution, $F(x)$ differs from its value at the solution by approximately one unit. This will usually imply that the Hessian matrix at the solution is well conditioned. It is unlikely that you will be able to follow these recommendations very closely, but it is worth trying (by guesswork), as sensible scaling will reduce the difficulty of the minimization problem, so that nag_opt_bounds_deriv (e04kbc) will take less computer time.

9.3 Unconstrained Minimization

If a problem is genuinely unconstrained and has been scaled sensibly, the following points apply:

(a) n_z will always be n,

(b) if **options.init_state** = Nag_Init_All or Nag_Init_H_S on entry, **options.state**$[j-1]$ has simply to be set to j, for $j = 1, 2, \ldots, n$,

(c) **options.hesl** and **options.hesd** will be factors of the full approximate second derivative matrix with elements stored in the natural order,

(d) the elements of **g** should all be close to zero at the final point,

(e) the `Status` values given in the printout from nag_opt_bounds_deriv (e04kbc) and in **options.state** on exit are unlikely to be of interest (unless they are negative, which would indicate that the modulus of one of the x_j has reached 10^{10} for some reason),

(f) `Norm g` simply gives the norm of the first derivative vector.

10 Example

This example minimizes the function

$$F = (x_1 + 10x_2)^2 + 5(x_3 - x_4)^2 + (x_2 - 2x_3)^4 + 10(x_1 - x_4)^4$$

subject to the bounds

$$\begin{aligned} 1 \leq x_1 \leq 3 \\ -2 \leq x_2 \leq 0 \\ 1 \leq x_4 \leq 3 \end{aligned}$$

starting from the initial guess $(3.0, -0.9, 0.13, 1.1)^{\mathrm{T}}$.

The **options** structure is declared and initialized by nag_opt_init (e04xxc). Four option values are read from a data file by use of nag_opt_read (e04xyc). The memory freeing function nag_opt_free (e04xzc) is used to free the memory assigned to the pointers in the option structure. You must **not** use the standard C function `free()` for this purpose.

10.1 Program Text

```
/* nag_opt_bounds_deriv (e04kbc) Example Program.
 *
 * Copyright 2014 Numerical Algorithms Group.
 *
 * Mark 2, 1991.
 * Mark 6 revised, 2000.
 * Mark 7, revised, 2001.
 * Mark 8 revised, 2004.
 *
 */

#include <nag.h>
#include <stdio.h>
#include <string.h>
#include <nag_stdlib.h>
#include <nage04.h>

#ifdef __cplusplus
extern "C" {
#endif
static void NAG_CALL objfun(Integer n, const double x[], double *f,
                            double g[], Nag_Comm *comm);
#ifdef __cplusplus
}
#endif

int main(void)
```

```
{
  const char    *optionsfile = "e04kbce.opt";
  Nag_Boolean   print;
  Integer       exit_status = 0;
  Integer       n;
  Nag_BoundType bound;
  Nag_E04_Opt   options;
  double        *bl = 0, *bu = 0, *g = 0, objf, *x = 0;
  Nag_Comm      comm;
  NagError      fail;

  INIT_FAIL(fail);

  printf("nag_opt_bounds_deriv (e04kbc) Example Program Results\n");
  fflush(stdout);

  n = 4;
  if (n >= 1)
    {
      if (!(x = NAG_ALLOC(n, double)) ||
          !(g = NAG_ALLOC(n, double)) ||
          !(bl = NAG_ALLOC(n, double)) ||
          !(bu = NAG_ALLOC(n, double)))
        {
          printf("Allocation failure\n");
          exit_status = -1;
          goto END;
        }
    }
  else
    {
      printf("Invalid n.\n");
      exit_status = 1;
      return exit_status;
    }

  x[0] = 3.0;
  x[1] = -0.9;
  x[2] = 0.13;
  x[3] = 1.1;

  /* Initialise options structure and read option values from file */
  print = Nag_TRUE;
  /* nag_opt_init (e04xxc).
   * Initialization function for option setting
   */
  nag_opt_init(&options);
#ifdef _WIN32
  strcpy_s(options.outfile, _countof(options.outfile), "stdout");
#else
  strcpy(options.outfile, "stdout");
#endif
  /* nag_opt_read (e04xyc).
   * Read options from a text file
   */
  nag_opt_read("e04kbc", optionsfile, &options, print, options.outfile, &fail);
  if (fail.code != NE_NOERROR)
    {
      printf("Error from nag_opt_read (e04xyc).\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
  bound = Nag_Bounds;
  bl[0] = 1.0;
  bu[0] = 3.0;
  bl[1] = -2.0;
  bu[1] = 0.0;
  /* Third variable is not bounded, so third lower bound
   * is set to a large negative number and third upper
   * bound to a large positive number.
   */
```

```
  bl[2] = -1.0e10;
  bu[2] = 1.0e10;
  bl[3] = 1.0;
  bu[3] = 3.0;

  /* nag_opt_bounds_deriv (e04kbc), see above. */
  nag_opt_bounds_deriv(n, objfun, bound, bl, bu, x, &objf,
                       g, &options, &comm, &fail);
  if (fail.code != NE_NOERROR)
    {
      printf("Error/Warning from nag_opt_bounds_deriv (e04kbc).\n%s\n",
             fail.message);
      if (fail.code != NW_COND_MIN)
        exit_status = 1;
    }

  /* Free memory allocated by nag_opt_bounds_deriv (e04kbc) to pointers hesd,
   * hesl and state.
   */
  /* nag_opt_free (e04xzc).
   * Memory freeing function for use with option setting
   */
  nag_opt_free(&options, "all", &fail);
  if (fail.code != NE_NOERROR)
    {
      printf("Error from nag_opt_free (e04xzc).\n%s\n", fail.message);
      exit_status = 3;
      goto END;
    }

 END:
  NAG_FREE(x);
  NAG_FREE(g);
  NAG_FREE(bl);
  NAG_FREE(bu);

  return exit_status;
}

static void NAG_CALL objfun(Integer n, const double x[], double *objf,
                            double g[], Nag_Comm *comm)
{
  /* Routine to evaluate objective function. */

  double x1, x2, x3, x4;
  double tmp, tmp1, tmp2, tmp3, tmp4;

  x1 = x[0];
  x2 = x[1];
  x3 = x[2];
  x4 = x[3];

  /* Supply a single function value */
  tmp1 = x1 + 10.0*x2;
  tmp2 = x3 - x4;
  tmp3 = x2 - 2.0*x3, tmp3 *= tmp3;
  tmp4 = x1 - x4, tmp4 *= tmp4;
  *objf = tmp1*tmp1 + 5.0*tmp2*tmp2 + tmp3*tmp3 + 10.0*tmp4*tmp4;

  if (comm->flag != 0)
    {
      tmp = x1 - x4;
      g[0] = 2.0*(x1 + 10.0*x2) + 40.0*tmp*tmp*tmp;
      tmp = x2 - 2.0*x3;
      g[1] = 20.0*(x1 + 10.0*x2) + 4.0*tmp*tmp*tmp;
      tmp = x2 - 2.0*x3;
      g[2] = 10.0*(x3 - x4) - 8.0*tmp*tmp*tmp;
      tmp = x1 - x4;
      g[3] = 10.0*(x4 - x3) - 40.0*tmp*tmp*tmp;
    }
}                               /* objfun */
```

10.2 Program Data

```
nag_opt_bounds_deriv (e04kbc) Example Program Optional Parameters

Following options for e04kbc are read by e04xyc.

begin e04kbc

print_level = Nag_Soln_Iter_Full /* Print full iterations and solution. */
max_iter = 40   /* Perform maximum of 40 iterations */
step_max = 4.0  /* Estimate minimum within 4 units of start */
f_est = 0.0     /* Zero is a lower bound on the function value */

end
```

10.3 Program Results

```
nag_opt_bounds_deriv (e04kbc) Example Program Results

Optional parameter setting for e04kbc.
--------------------------------------

Option file: e04kbce.opt

print_level set to Nag_Soln_Iter_Full
max_iter set to 40
step_max set to 4.00e+00
f_est set to 0.00e+00

Parameters to e04kbc
--------------------

Number of variables...........   4

optim_tol...............  1.05e-07    linesearch_tol..........  9.00e-01
f_est...................  0.00e+00
step_max................  4.00e+00    max_iter................        40
init_state.......... Nag_Init_None    local_search............      Nag_TRUE
minlin.............. Nag_Lin_Deriv    deriv_check.............      Nag_TRUE
print_level.... Nag_Soln_Iter_Full    machine precision.......  1.11e-16
outfile.................    stdout

Memory allocation:
state...................       Nag
hesl....................       Nag    hesd...................        Nag

Results from e04kbc:
-------------------

Iteration results:

  Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
   0     0   1.7284e+02   2.9e+02   3.3e+00                            1.0e+00

 Variable         x               g          Status
    1         3.0000e+00       2.6236e+02    Upper Bound
    2        -9.0000e-01      -1.2624e+02    Free
    3         1.3000e-01       2.7872e+00    Free
    4         1.1000e+00      -2.6466e+02    Free

  Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
   1     1   2.6813e+01   2.7e+01   3.7e+00     1.2e+00      4.0e-03   3.4e+01

 Variable         x               g          Status
    1         3.0000e+00       2.1529e+01    Upper Bound
    2        -3.9251e-01      -1.9503e+01    Free
    3         1.1880e-01      -1.8450e+01    Free
    4         2.1639e+00      -2.9276e+00    Free

  Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
```

```
  2     3   2.3453e+01   2.0e+01   3.7e+00     2.6e-01      1.0e-02   4.2e+01

 Variable        x               g          Status
    1         3.0000e+00      2.9429e+01    Upper Bound
    2        -2.2652e-01      1.2204e+01    Free
    3         3.1377e-01     -1.3004e+01    Free
    4         2.1125e+00     -9.9713e+00    Free

  Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
   3     6   2.1599e+01   2.8e+01   3.7e+00     2.2e-01      8.7e-03   2.3e+02

 Variable        x               g          Status
    1         3.0000e+00      2.6022e+01    Free
    2        -2.5718e-01     -6.5438e-01    Free
    3         5.3184e-01      2.3232e+00    Free
    4         2.1431e+00     -9.0525e+00    Free

  Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
   4     8   1.6189e+01   2.3e+01   3.1e+00     8.0e-01      3.1e-02   8.9e+00

 Variable        x               g          Status
    1         2.1985e+00     -7.4626e-01    Free
    2        -2.5748e-01     -1.6715e+01    Free
    3         5.3101e-01      2.2448e+00    Free
    4         2.1444e+00      1.6128e+01    Free

  Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
   5     9   1.4024e+01   1.5e+01   3.0e+00     1.7e-01      1.0e+00   1.8e+01

 Variable        x               g          Status
    1         2.0816e+00      7.7589e-01    Free
    2        -1.6942e-01      8.3975e-01    Free
    3         5.1518e-01     -1.5466e+00    Free
    4         2.0515e+00      1.5362e+01    Free

  Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
   6    10   1.1240e+01   2.1e+01   2.6e+00     3.8e-01      1.0e+00   5.4e+01

 Variable        x               g          Status
    1         1.7877e+00      2.1366e+00    Free
    2        -7.1798e-02      1.5908e+01    Free
    3         5.1964e-01     -2.1209e+00    Free
    4         1.8290e+00      1.3096e+01    Free

  Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
   7    11   7.9843e+00   1.1e+01   2.1e+00     5.4e-01      6.2e-01   3.9e+00

 Variable        x               g          Status
    1         1.3605e+00      2.5858e+00    Free
    2         0.0000e+00      2.3422e+01    Upper Bound
    3         4.9104e-01     -2.6186e+00    Free
    4         1.5106e+00      1.0331e+01    Free

  Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
   8    12   5.3035e+00   9.3e+00   1.7e+00     3.7e-01      1.0e+00   1.1e+01

 Variable        x               g          Status
    1         1.0732e+00      1.7792e+00    Free
    2         0.0000e+00      1.8627e+01    Upper Bound
    3         4.4590e-01     -2.6928e+00    Free
    4         1.2826e+00      8.7338e+00    Free

  Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
   9    13   4.6913e+00   1.9e+01   1.6e+00     9.5e-02      6.6e-02   7.3e+01

 Variable        x               g          Status
    1         1.0000e+00      1.5613e+00    Lower Bound
    2         0.0000e+00      1.7336e+01    Free
    3         4.3666e-01     -2.5266e+00    Free
    4         1.2222e+00      8.2939e+00    Free
```

```
 Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
 10    15   3.9688e+00   8.3e+00   1.6e+00     8.3e-02      4.8e-03   3.9e+00

Variable        x               g          Status
   1         1.0000e+00      -9.4589e-02    Lower Bound
   2        -8.3009e-02      -1.0146e-01    Free
   3         4.3672e-01      -8.4789e-01    Free
   4         1.2215e+00       8.2818e+00    Free

 Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
 11    16   2.8304e+00   6.4e+00   1.5e+00     1.6e-01      1.0e+00   1.9e+01

Variable        x               g          Status
   1         1.0000e+00       3.1074e-01    Lower Bound
   2        -8.3930e-02      -3.6206e-02    Free
   3         4.2460e-01       1.0297e-01    Free
   4         1.0643e+00       6.4079e+00    Free

 Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
 12    17   2.4344e+00   2.4e-01   1.5e+00     6.5e-02      1.1e-01   2.6e+00

Variable        x               g          Status
   1         1.0000e+00       3.0156e-01    Lower Bound
   2        -8.4922e-02      -3.4052e-02    Free
   3         4.1431e-01       2.4239e-01    Free
   4         1.0000e+00       5.8569e+00    Lower Bound

 Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
 13    18   2.4339e+00   8.7e-02   1.5e+00     3.2e-03      1.0e+00   4.1e+00

Variable        x               g          Status
   1         1.0000e+00       2.9879e-01    Lower Bound
   2        -8.5060e-02      -7.5964e-05    Free
   3         4.1114e-01       8.7488e-02    Free
   4         1.0000e+00       5.8886e+00    Lower Bound

 Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
 14    19   2.4338e+00   7.8e-04   1.5e+00     1.8e-03      1.0e+00   4.1e+00

Variable        x               g          Status
   1         1.0000e+00       2.9535e-01    Lower Bound
   2        -8.5233e-02      -2.7717e-04    Free
   3         4.0932e-01       7.2996e-04    Free
   4         1.0000e+00       5.9068e+00    Lower Bound

 Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
 15    20   2.4338e+00   3.5e-06   1.5e+00     1.5e-05      1.0e+00   4.1e+00

Variable        x               g          Status
   1         1.0000e+00       2.9535e-01    Lower Bound
   2        -8.5233e-02      -2.5483e-06    Free
   3         4.0930e-01       2.3869e-06    Free
   4         1.0000e+00       5.9070e+00    Lower Bound

 Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
 16    21   2.4338e+00   8.2e-09   1.5e+00     4.6e-08      1.0e+00   4.1e+00

Variable        x               g          Status
   1         1.0000e+00       2.9535e-01    Lower Bound
   2        -8.5233e-02      -8.1823e-09    Free
   3         4.0930e-01       1.0494e-10    Free
   4         1.0000e+00       5.9070e+00    Lower Bound

 Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
 17    22   2.4338e+00   8.2e-09   1.5e+00     4.2e-11      1.0e+00   1.0e+00

Variable        x               g          Status
   1         1.0000e+00       2.9535e-01    Lower Bound
   2        -8.5233e-02      -8.1823e-09    Free
   3         4.0930e-01       1.0494e-10    Free
   4         1.0000e+00       5.9070e+00    Lower Bound
```

```
  Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
  18    23   2.4338e+00   8.2e-09   1.5e+00     4.2e-11      1.0e+00   1.0e+00

 Variable        x              g          Status
    1         1.0000e+00      2.9535e-01    Lower Bound
    2        -8.5233e-02     -8.1823e-09    Free
    3         4.0930e-01      1.0494e-10    Free
    4         1.0000e+00      5.9070e+00    Lower Bound

Local search performed.

Final solution:

  Itn  Nfun  Objective    Norm g    Norm x  Norm(x(k-1)-x(k))  Step    Cond H
  18    27   2.4338e+00   8.2e-09   1.5e+00     8.2e-09      1.0e+00   1.0e+00

 Variable        x              g          Status
    1         1.0000e+00      2.9535e-01    Lower Bound
    2        -8.5233e-02     -8.1823e-09    Free
    3         4.0930e-01      1.0494e-10    Free
    4         1.0000e+00      5.9070e+00    Lower Bound
Error/Warning from nag_opt_bounds_deriv (e04kbc).
NW_COND_MIN:
  The conditions for a minimum have not all been satisfied but a lower
  point could not be found.
```

11 Optional Arguments

A number of optional input and output arguments to nag_opt_bounds_deriv (e04kbc) are available through the structure argument **options**, type Nag_E04_Opt. An argument may be selected by assigning an appropriate value to the relevant structure member; those arguments not selected will be assigned default values. If no use is to be made of any of the optional arguments you should use the NAG defined null pointer, `E04_DEFAULT`, in place of **options** when calling nag_opt_bounds_deriv (e04kbc); the default settings will then be used for all arguments.

Before assigning values to **options** directly the structure **must** be initialized by a call to the function nag_opt_init (e04xxc). Values may then be assigned to the structure members in the normal C manner.

Option settings may also be read from a text file using the function nag_opt_read (e04xyc) in which case initialization of the **options** structure will be performed automatically if not already done. Any subsequent direct assignment to the **options** structure must **not** be preceded by initialization.

If assignment of functions and memory to pointers in the **options** structure is required, then this must be done directly in the calling program; they cannot be assigned using nag_opt_read (e04xyc).

11.1 Optional Argument Checklist and Default Values

For easy reference, the following list shows the members of **options** which are valid for nag_opt_bounds_deriv (e04kbc) together with their default values where relevant. The number ϵ is a generic notation for ***machine precision*** (see nag_machine_precision (X02AJC)).

`Boolean list`	Nag_TRUE
`Nag_PrintType print_level`	**Nag_Soln_Iter**
`char outfile[80]`	`stdout`
`void (*print_fun)()`	**NULL**
`Boolean deriv_check`	Nag_TRUE
`Nag_InitType init_state`	**Nag_Init_None**
`Integer max_iter`	50**n**
`double optim_tol`	$10\sqrt{\epsilon}$
`Nag_LinFun minlin`	**Nag_Lin_Deriv**
`double linesearch_tol`	0.9 (0.0 if $\mathbf{n} = 1$)
`double step_max`	100000.0
`double f_est`	

`Boolean local_search`	Nag_TRUE
`Integer *state`	size **n**
`double *hesl`	size $\max(\mathbf{n}[\mathbf{n}-1]/2, 1)$
`double *hesd`	size **n**
`Integer iter`	
`Integer nf`	

11.2 Description of the Optional Arguments

list – Nag_Boolean Default $=$ Nag_TRUE

On entry: if **options.list** $=$ Nag_TRUE the argument settings in the call to nag_opt_bounds_deriv (e04kbc) will be printed.

print_level – Nag_PrintType Default $=$ Nag_Soln_Iter

On entry: the level of results printout produced by nag_opt_bounds_deriv (e04kbc). The following values are available:

Nag_NoPrint	No output.
Nag_Soln	The final solution.
Nag_Iter	One line of output for each iteration.
Nag_Soln_Iter	The final solution and one line of output for each iteration.
Nag_Soln_Iter_Full	The final solution and detailed printout at each iteration.

Details of each level of results printout are described in Section 11.3.

Constraint: **options.print_level** $=$ Nag_NoPrint, Nag_Soln, Nag_Iter, Nag_Soln_Iter or Nag_Soln_Iter_Full.

outfile – const char[80] Default $=$ `stdout`

On entry: the name of the file to which results should be printed. If **options.outfile**[0] $=$ '\0' then the `stdout` stream is used.

print_fun – pointer to function Default $=$ **NULL**

On entry: printing function defined by you; the prototype of **options.print_fun** is

```
void (*print_fun)(const Nag_Search_State *st, Nag_Comm *comm);
```

See Section 11.3.1 below for further details.

deriv_check – Nag_Boolean Default $=$ Nag_TRUE

If **options.init_state** $\neq$ Nag_Init_None then the default of **options.deriv_check** is changed to Nag_FALSE.

On entry: if **options.deriv_check** $=$ Nag_TRUE a check of the derivatives defined by **objfun** will be made at the starting point **x**. The derivative check is carried out by a call to nag_opt_check_deriv (e04hcc). If **options.init_state** is set to a value other than its default value (**options.init_state** $=$ Nag_Init_None) then the default of **options.deriv_check** will be Nag_FALSE. A starting point of $x = 0$ or $x = 1$ should be avoided if this test is to be meaningful, if either of these starting points is necessary then nag_opt_check_deriv (e04hcc) should be used to check **objfun** at a different point prior to calling nag_opt_bounds_deriv (e04kbc).

init_state – Nag_InitType Default $=$ Nag_Init_None

On entry: **options.init_state** specifies which of the arguments **objf**, **g**, **options.hesl**, **options.hesd** and **options.state** are actually being initialized. Such information will generally reduce the time taken by nag_opt_bounds_deriv (e04kbc).

options.init_state $=$ Nag_Init_None
No values are assumed to have been set in any of **objf**, **g**, **options.hesl**, **options.hesd** or **options.state**. (nag_opt_bounds_deriv (e04kbc) will use the unit matrix as the initial estimate of the Hessian matrix.)

options.init_state $=$ Nag_Init_F_G_H
The arguments **objf** and **g** must contain the value of $F(x)$ and its first derivatives at the starting point. The elements **options.hesd**$[j-1]$ must have been set to estimates of the derivatives $\dfrac{\partial^2 F}{\partial x_j^2}$ at the starting point. No values are assumed to have been set in **options.hesl** or **options.state**.

options.init_state $=$ Nag_Init_All
The arguments **objf** and **g** must contain the value of $F(x)$ and its first derivatives at the starting point. All n elements of **options.state** must have been set to indicate which variables are on their bounds and which are free. **options.hesl** and **options.hesd** must contain the Cholesky factors of a positive definite approximation to the n_z by n_z Hessian matrix for the subspace of free variables. (This option is useful for restarting the minimization process if **options.max_iter** is reached.)

options.init_state $=$ Nag_Init_H_S
No values are assumed to have been set in **objf** or **g**, but **options.hesl**, **options.hesd** and **options.state** must have been set as for **options.init_state** $=$ Nag_Init_All. (This option is useful for starting off a minimization run using second derivative information from a previous, similar, run.)

Constraint: **options.init_state** $=$ Nag_Init_None, Nag_Init_F_G_H, Nag_Init_All or Nag_Init_H_S.

max_iter – Integer Default $= 50$**n**

On entry: the limit on the number of iterations allowed before termination.

Constraint: **options.max_iter** ≥ 0.

optim_tol – double Default $= 10\sqrt{\epsilon}$

On entry: the accuracy in x to which the solution is required. If x_{true} is the true value of x at the minimum, then x_{sol}, the estimated position prior to a normal exit, is such that

$$\|x_{\text{sol}} - x_{\text{true}}\| < \textbf{options.optim\_tol} \times (1.0 + \|x_{\text{true}}\|),$$

where $\|y\| = \left(\sum_{j=1}^n y_j^2\right)^{1/2}$. For example, if the elements of x_{sol} are not much larger than 1.0 in modulus and if **options.optim_tol** is set to 10^{-5}, then x_{sol} is usually accurate to about 5 decimal places. (For further details see Section 9.) If the problem is scaled roughly as described in Section 9 and ϵ is the ***machine precision***, then $\sqrt{\epsilon}$ is probably the smallest reasonable choice for **options.optim_tol**. (This is because, normally, to machine accuracy, $F\left(x + \sqrt{\epsilon}e_j\right) = F(x)$ where e_j is any column of the identity matrix.)

Constraint: $\epsilon \leq$ **options.optim_tol** < 1.0.

minlin – Nag_LinFun Default $=$ Nag_Lin_Deriv

On entry: **options.minlin** specifies whether the linear minimizations (i.e., minimizations of $F(x + \alpha p)$ with respect to α) are to be performed by a function which just requires the evaluation of $F(x)$, Nag_Lin_NoDeriv, or by a function which also requires the first derivatives of $F(x)$, Nag_Lin_Deriv.

It will often be possible to evaluate the first derivatives of F in about the same amount of computer time that is required for the evaluation of F itself – if this is so then nag_opt_bounds_deriv (e04kbc) should be called with **options.minlin** set to Nag_Lin_Deriv. However, if the evaluation of the derivatives takes more than about 4 times as long as the evaluation of F, then a setting of Nag_Lin_NoDeriv will usually be preferable. If in doubt, use the default setting Nag_Lin_Deriv as it is slightly more robust.

Constraint: **options.minlin** = Nag_Lin_Deriv or Nag_Lin_NoDeriv.

linesearch_tol – double Default $= 0.9$ if $\mathbf{n} > 1$, and 0.0 otherwise

If **options.minlin** = Nag_Lin_NoDeriv then the default value of **options.linesearch_tol** will be changed from 0.9 to 0.5 if $\mathbf{n} > 1$.

On entry: every iteration of nag_opt_bounds_deriv (e04kbc) involves a linear minimization (i.e., minimization of $F(x + \alpha p)$ with respect to α). **options.linesearch_tol** specifies how accurately these linear minimizations are to be performed. The minimum with respect to α will be located more accurately for small values of **options.linesearch_tol** (say 0.01) than for large values (say 0.9).

Although accurate linear minimizations will generally reduce the number of iterations performed by nag_opt_bounds_deriv (e04kbc), they will increase the number of function evaluations required for each iteration. On balance, it is usually more efficient to perform a low accuracy linear minimization.

A smaller value such as 0.01 may be worthwhile:

(a) if **objfun** takes so little computer time that it is worth using extra calls of **objfun** to reduce the number of iterations and associated matrix calculations

(b) if $F(x)$ is a penalty or barrier function arising from a constrained minimization problem (since such problems are very difficult to solve)

(c) if **options.minlin** = Nag_Lin_NoDeriv and the calculation of first derivatives takes so much computer time (relative to the time taken to evaluate the function) that it is worth using extra function evaluations to reduce the number of derivative evaluations.

If $\mathbf{n} = 1$, the default for **options.linesearch_tol** = 0.0 (if the problem is effectively one-dimensional then **options.linesearch_tol** should be set to 0.0 even though $\mathbf{n} > 1$; i.e., if for all except one of the variables the lower and upper bounds are equal).

Constraint: $0.0 \leq$ **options.linesearch_tol** < 1.0.

step_max – double Default $= 100000.0$

On entry: an estimate of the Euclidean distance between the solution and the starting point supplied. (For maximum efficiency a slight overestimate is preferable.) nag_opt_bounds_deriv (e04kbc) will ensure that, for each iteration,

$$\left(\sum_{j=1}^{n}\left[x_j^{(k)} - x_j^{(k-1)}\right]^2\right)^{1/2} \leq \mathbf{options.step\_max},$$

where k is the iteration number. Thus, if the problem has more than one solution, nag_opt_bounds_deriv (e04kbc) is most likely to find the one nearest the starting point. On difficult problems, a realistic choice can prevent the sequence of $x^{(k)}$ entering a region where the problem is ill-behaved and can also help to avoid possible overflow in the evaluation of $F(x)$. However an underestimate of **options.step_max** can lead to inefficiency.

Constraint: **options.step_max** $\geq$ **options.optim_tol**.

f_est – double

On entry: an estimate of the function value at the minimum. This estimate is just used for calculating suitable step lengths for starting linear minimizations off, so the choice is not too critical. However, it is better for **options.f_est** to be set to an underestimate rather than to an overestimate. If no value is supplied then an initial step length of 1.0, subject to the variable bounds, will be used.

local_search – Nag_Boolean Default = Nag_TRUE

On entry: **options.local_search** must specify whether or not you wish a ‘local search’ to be performed when a point is found which is thought to be a constrained minimum.

If **options**.**local_search** = Nag_TRUE and either the quasi-Newton direction of search fails to produce a lower function value or the convergence criteria are satisfied, then a local search will be performed. This may move the search away from a saddle point or confirm that the final point is a minimum.

If **options**.**local_search** = Nag_FALSE there will be no local search when a point is found which is thought to be a minimum.

The amount of work involved in a local search is comparable to twice that required in a normal iteration to minimize $F(x + \alpha p)$ with respect to α. For most problems this will be small (relative to the total time required for the minimization). **options**.**local_search** could be set Nag_FALSE if:

– it is known from the physical properties of a problem that a stationary point will be the required minimum;

– a point which is not a minimum could be easily recognized, for example if the value of $F(x)$ at the minimum is known.

state – Integer * Default memory $=$ **n**

On entry: **options**.**state** need not be set if the default option of **options**.**init_state** = Nag_Init_None is used as **n** values of memory will be automatically allocated by nag_opt_bounds_deriv (e04kbc).

If **options**.**init_state** = Nag_Init_All or Nag_Init_H_S has been chosen, **options**.**state** must point to a minimum of **n** elements of memory. This memory will already be available if the calling program has used the **options** structure in a previous call to nag_opt_bounds_deriv (e04kbc) with **options**.**init_state** = Nag_Init_None and the same value of **n**. If a previous call has not been made you must allocate sufficient memory.

When **options**.**init_state** = Nag_Init_All or Nag_Init_H_S then **options**.**state** must specify information about which variables are currently on their bounds and which are free. If x_j is:

(a) fixed on its upper bound, **options**.**state**$[j-1]$ is -1;

(b) fixed on its lower bound, **options**.**state**$[j-1]$ is -2;

(c) effectively a constant (i.e., $l_j = u_j$), **options**.**state**$[j-1]$ is -3;

(d) free, **options**.**state**$[j-1]$ gives its position in the sequence of free variables.

If **options**.**init_state** = Nag_Init_None or Nag_Init_F_G_H, **options**.**state** will be initialized by nag_opt_bounds_deriv (e04kbc).

If **options**.**init_state** = Nag_Init_All or Nag_Init_H_S, **options**.**state** must be initialized before nag_opt_bounds_deriv (e04kbc) is called.

On exit: **options**.**state** gives information as above about the final point given in **x**.

hesl – double * Default memory $= \max(\mathbf{n}[\mathbf{n}-1]/2, 1)$
hesd – double * Default memory $=$ **n**

On entry: **options**.**hesl** and **options**.**hesd** need not be set if the default of **options**.**init_state** = Nag_Init_None is used as sufficient memory will be automatically allocated by nag_opt_bounds_deriv (e04kbc).

If **options**.**init_state** = Nag_Init_All or **options**.**init_state** = Nag_Init_H_S has been set then **options**.**hesl** must point to a minimum of $\max(\mathbf{n}[\mathbf{n}-1]/2, 1)$ elements of memory.

options.**hesd** must point to at least **n** elements of memory if **options**.**init_state** = Nag_Init_F_G_H, Nag_Init_All or Nag_Init_H_S has been chosen.

The appropriate amount of memory will already be available for **options**.**hesl** and **options**.**hesd** if the calling program has used the **options** structure in a previous call to nag_opt_bounds_deriv (e04kbc) with **options**.**init_state** = Nag_Init_None and the same value of **n**. If a previous call has not been made, you must allocate sufficient memory.

options.**hesl** and **options**.**hesd** are used to store the factors L and D of the current approximation to the matrix of second derivatives with respect to the free variables (see Section 3). (The elements of the matrix are assumed to be ordered according to the permutation specified by the positive elements of

options.state, see above.) **options.hesl** holds the lower triangle of L, omitting the unit diagonal, stored by rows. **options.hesd** stores the diagonal elements of D. Thus if n_z elements of **options.state** are positive, the strict lower triangle of L will be held in the first $n_z(n_z - 1)/2$ elements of **options.hesl** and the diagonal elements of D in the first n_z elements of **options.hesd**.

If **options.init_state** $=$ Nag_Init_None (the default), **options.hesl** and **options.hesd** will be initialized within nag_opt_bounds_deriv (e04kbc) to the factors of the unit matrix.

If you set **options.init_state** $=$ Nag_Init_F_G_H, **options.hesd**$[j-1]$ must contain on entry an approximation to the second derivative with respect to x_j, for $j = 1, 2, \ldots, n$. **options.hesl** need not be set.

If **options.init_state** $=$ Nag_Init_All or Nag_Init_H_S, **options.hesl** and **options.hesd** must contain on entry the Cholesky factors of a positive definite approximation to the n_z by n_z matrix of second derivatives for the subspace of free variables as specified by your setting of **options.state**.

On exit: **options.hesl** and **options.hesd** hold the factors L and D corresponding to the final point given in **x**. The elements of **options.hesd** are useful for deciding whether to accept the result produced by nag_opt_bounds_deriv (e04kbc) (see Section 9).

iter – Integer

On exit: the number of iterations which have been performed in nag_opt_bounds_deriv (e04kbc).

nf – Integer

On exit: the number of times the residuals have been evaluated (i.e., number of calls of **objfun**).

11.3 Description of Printed Output

The level of printed output can be controlled with the structure members **options.list** and **options.print_level** (see Section 11.2). If **options.list** $=$ Nag_TRUE then the argument values to nag_opt_bounds_deriv (e04kbc) are listed, whereas the printout of results is governed by the value of **options.print_level**. The default of **options.print_level** $=$ Nag_Soln_Iter provides a single line of output at each iteration and the final result. This section describes all of the possible levels of results printout available from nag_opt_bounds_deriv (e04kbc).

When **options.print_level** $=$ Nag_Iter or Nag_Soln_Iter a single line of output is produced on completion of each iteration, this gives the following values:

`Itn`	the iteration count, k.
`Nfun`	the cumulative number of calls to **objfun**.
`Objective`	the current value of the objective function, $F\left(x^{(k)}\right)$
`Norm g`	the Euclidean norm of the projected gradient vector, $\left\|g_z\left(x^{(k)}\right)\right\|$.
`Norm x`	the Euclidean norm of $x^{(k)}$.
`Norm(x(k-1)-x(k))`	the Euclidean norm of $x^{(k-1)} - x^{(k)}$.
`Step`	the step $\alpha^{(k)}$ taken along the computed search direction $p^{(k)}$.
`Cond H`	the ratio of the largest to the smallest element of the diagonal factor D of the projected Hessian matrix. This quantity is usually a good estimate of the condition number of the projected Hessian matrix. (If no variables are currently free, this value will be zero.)

When **options.print_level** $=$ Nag_Soln_Iter_Full more detailed results are given at each iteration. Additional values output are:

`x`	the current point $x^{(k)}$.
`g`	the current projected gradient vector, $g_z\left(x^{(k)}\right)$.
`Status`	the current state of the variable with respect to its bound(s).

If **options.print_level** $=$ Nag_Soln, Nag_Soln_Iter or Nag_Soln_Iter_Full the final result is printed out. This consists of:

`x`	the final point, x^*.
`g`	the final projected gradient vector, $g_z(x^*)$.
`Status`	the final state of the variable with respect to its bound(s).

If **options.print_level** = Nag_NoPrint then printout will be suppressed; you can print the final solution when nag_opt_bounds_deriv (e04kbc) returns to the calling program.

11.3.1 Output of results via a user-defined printing function

You may also specify your own print function for output of iteration results and the final solution by use of the **options.print_fun** function pointer, which has prototype

The rest of this section can be skipped if the default printing facilities provide the required functionality.

When a user-defined function is assigned to **options.print_fun** this will be called in preference to the internal print function of nag_opt_bounds_deriv (e04kbc). Calls to the user-defined function are again controlled by means of the **options.print_level** member. Information is provided through **st** and **comm**, the two structure arguments to **options.print_fun**.

The results contained in the members of **st** are those on completion of the last iteration or those after a local search. (An iteration may be followed by a local search (see **options.local_search**, Section 11.2) in which case **options.print_fun** is called with the results of the last iteration (**st→local_search** = Nag_FALSE) and then again when the local search has been completed (**st→local_search** = Nag_TRUE).)

If **comm→it_prt** = Nag_TRUE then the results on completion of an iteration of nag_opt_bounds_deriv (e04kbc) are contained in the members of **st**. If **comm→sol_prt** = Nag_TRUE then the final results from nag_opt_bounds_deriv (e04kbc), including details of the final iteration, are contained in the members of **st**. In both cases, the same members of **st** are set, as follows:

iter – Integer

The current iteration count, k, if **comm→it_prt** = Nag_TRUE; the final iteration count, k, if **comm→sol_prt** = Nag_TRUE.

n – Integer

The number of variables.

x – double *

The coordinates of the point $x^{(k)}$.

f – double *

The value of the current objective function.

g – double *

Points to the **n** memory locations holding the first derivatives of F at the current point $x^{(k)}$.

gpj_norm – double *

The Euclidean norm of the current projected gradient g_z.

step – double *

The step $\alpha^{(k)}$ taken along the search direction $p^{(k)}$.

cond – double *

The estimate of the condition number of the Hessian matrix.

xk_norm – double *

The Euclidean norm of $x^{(k-1)} - x^{(k)}$.

state – Integer

The status of variables x_j, $j = 1, 2, \ldots, n$, with respect to their bounds. See Section 3 for a description of the possible status values.

local_search – Nag_Boolean

Nag_TRUE if a local search has been performed.

nf – Integer

The cumulative number of calls made to **objfun**.

The relevant members of the structure **comm** are:

it_prt – Nag_Boolean

Will be Nag_TRUE when the print function is called with the results of the current iteration.

sol_prt – Nag_Boolean

Will be Nag_TRUE when the print function is called with the final result.

user – double *
iuser – Integer *
p – Pointer

Pointers for communication of user information. If used they must be allocated memory either before entry to nag_opt_bounds_deriv (e04kbc) or during a call to **objfun** or **options.print_fun**. The type Pointer will be `void *` with a C compiler that defines `void *` and `char *` otherwise.