NAG Library Function Document

nag_opt_nlp_solve (e04wdc)

Note: *this function uses* **optional arguments** *to define choices in the problem specification and in the details of the algorithm. If you wish to use* default *settings for all of the optional arguments, you need only read Sections 1 to 10 of this document. If, however, you wish to reset some or all of the settings please refer to Section 11 for a detailed description of the algorithm, to Section 12 for a detailed description of the specification of the optional arguments and to Section 13 for a detailed description of the monitoring information produced by the function.*

1 Purpose

nag_opt_nlp_solve (e04wdc) is designed to minimize an arbitrary smooth function subject to constraints (which may include simple bounds on the variables, linear constraints and smooth nonlinear constraints) using a sequential quadratic programming (SQP) method. As many first derivatives as possible should be supplied by you; any unspecified derivatives are approximated by finite differences. It is not intended for large sparse problems.

nag_opt_nlp_solve (e04wdc) may also be used for unconstrained, bound-constrained and linearly constrained optimization.

nag_opt_nlp_solve (e04wdc) uses **forward communication** for evaluating the objective function, the nonlinear constraint functions, and any of their derivatives.

The initialization function nag_opt_nlp_init (e04wcc) **must** have been called before to calling nag_opt_nlp_solve (e04wdc).

2 Specification

```
#include <nag.h>
#include <nage04.h>
void nag_opt_nlp_solve (Integer n, Integer nclin, Integer ncnln, Integer tda,
     Integer tdcj, Integer tdh, const double a[], const double bl[],
     const double bu[],
     void (*confun)(Integer *mode, Integer ncnln, Integer n, Integer tdcj,
          const Integer needc[], const double x[], double ccon[],
          double cjac[], Integer nstate, Nag_Comm *comm),
     void (*objfun)(Integer *mode, Integer n, const double x[], double *objf,
          double grad[], Integer nstate, Nag_Comm *comm),
     Integer *majits, Integer istate[], double ccon[], double cjac[],
     double clamda[], double *objf, double grad[], double h[], double x[],
     Nag_E04State *state, Nag_Comm *comm, NagError *fail)
```

Before calling nag_opt_nlp_solve (e04wdc), or any of the option setting functions nag_opt_nlp_option_set_file (e04wec), nag_opt_nlp_option_set_string (e04wfc), nag_opt_nlp_option_set_integer (e04wgc) or nag_opt_nlp_option_set_double (e04whc), nag_opt_nlp_init (e04wcc) **must** be called. The specification for nag_opt_nlp_init (e04wcc) is:

```
#include <nag.h>
#include <nage04.h>
void nag_opt_nlp_init (Nag_E04State *state, NagError *fail)
```

The contents of **state must not** be altered between calls of the functions nag_opt_nlp_init (e04wcc), nag_opt_nlp_solve (e04wdc), nag_opt_nlp_option_set_file (e04wec), nag_opt_nlp_option_set_integer (e04wgc) or nag_opt_nlp_option_set_double (e04whc).

3 Description

nag_opt_nlp_solve (e04wdc) is designed to solve nonlinear programming problems – the minimization of a smooth nonlinear function subject to a set of constraints on the variables. nag_opt_nlp_solve (e04wdc) is suitable for small dense problems. The problem is assumed to be stated in the following form:

$$\underset{x \in R^n}{\text{minimize}} F(x) \quad \text{subject to} \quad l \leq \begin{pmatrix} x \\ A_L x \\ c(x) \end{pmatrix} \leq u, \tag{1}$$

where $F(x)$ (the *objective function*) is a nonlinear scalar function, A_L is an n_L by n constant matrix, and $c(x)$ is an n_N-vector of nonlinear constraint functions. (The matrix A_L and the vector $c(x)$ may be empty.) The objective function and the constraint functions are assumed to be smooth, here meaning at least twice-continuously differentiable. (The method of nag_opt_nlp_solve (e04wdc) will usually solve (1) if there are only isolated discontinuities away from the solution.) We also write $r(x)$ for the vector of combined functions:

$$r(x) = \begin{pmatrix} x & A_L x & c(x) \end{pmatrix}^{\mathrm{T}}.$$

Note that although the bounds on the variables could be included in the definition of the linear constraints, we prefer to distinguish between them for reasons of computational efficiency. For the same reason, the linear constraints should **not** be included in the definition of the nonlinear constraints. Upper and lower bounds are specified for all the variables and for all the constraints. An *equality* constraint on r_i can be specified by setting $l_i = u_i$. If certain bounds are not present, the associated elements of l or u can be set to special values that will be treated as $-\infty$ or $+\infty$. (See the description of the optional argument **Infinite Bound Size**.)

A typical invocation of nag_opt_nlp_solve (e04wdc) is:

```
nag_opt_nlp_init(&state, ...);
nag_opt_nlp_option_set_file(ispecs, &state, ...);
nag_opt_nlp_solve(n, nclin, ncnln, ...);
```

where nag_opt_nlp_option_set_file (e04wec) reads a file of optional definitions.

Figure 1 illustrates the feasible region for the jth pair of constraints $l_j \leq r_j(x) \leq u_j$. The quantity of δ is the **Feasibility Tolerance**, which can be set by you (see Section 12). The constraints $l_j \leq r_j \leq u_j$ are considered 'satisfied' if r_j lies in Regions 2, 3 or 4, and 'inactive' if r_j lies in Region 3. The constraint $r_j \geq l_j$ is considered 'active' in Region 2, and 'violated' in Region 1. Similarly, $r_j \leq u_j$ is active in Region 4, and violated in Region 5. For equality constraints ($l_j = u_j$), Regions 2 and 4 are the same and Region 3 is empty.

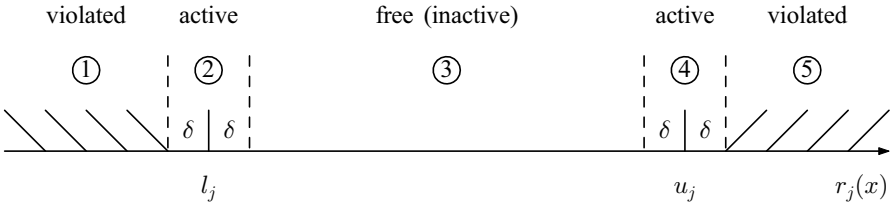

Figure 1
Illustration of the constraints $l_j \leq r_j(x) \leq u_j$

If there are no nonlinear constraints in (1) and F is linear or quadratic, then it will generally be more efficient to use one of nag_opt_lp (e04mfc), nag_opt_lin_lsq (e04ncc) or nag_opt_qp (e04nfc). If the problem is large and sparse and does have nonlinear constraints, then nag_opt_sparse_nlp_solve (e04vhc) should be used, since nag_opt_nlp_solve (e04wdc) treats all matrices as dense.

You must supply an initial estimate of the solution to (1), together with functions that define $F(x)$ and $c(x)$ with as many first partial derivatives as possible; unspecified derivatives are approximated by finite differences; see Section 12.1 for a discussion of the optional argument **Derivative Level**.

The objective function is defined by **objfun**, and the nonlinear constraints are defined by **confun**. Note that if there *are* any nonlinear constraints then the *first* call to **confun** will precede the *first* call to **objfun**.

For maximum reliability, it is preferable for you to provide all partial derivatives (see Chapter 8 of Gill *et al.* (1981), for a detailed discussion). If all gradients cannot be provided, it is similarly advisable to provide as many as possible. While developing **objfun** and **confun**, the optional argument **Verify Level** should be used to check the calculation of any known gradients.

The method used by nag_opt_nlp_solve (e04wdc) is based on NPOPT, which is part of the SNOPT package described in Gill *et al.* (2005b), and the algorithm it uses is described in detail in Section 11.

4 References

Eldersveld S K (1991) Large-scale sequential quadratic programming algorithms *PhD Thesis* Department of Operations Research, Stanford University, Stanford

Fourer R (1982) Solving staircase linear programs by the simplex method *Math. Programming* **23** 274–313

Gill P E, Murray W and Saunders M A (2002) *SNOPT: An SQP Algorithm for Large-scale Constrained Optimization* **12** 979–1006 SIAM J. Optim.

Gill P E, Murray W and Saunders M A (2005a) Users' guide for SQOPT 7: a Fortran package for large-scale linear and quadratic programming *Report NA 05-1* Department of Mathematics, University of California, San Diego http://www.ccom.ucsd.edu/~peg/papers/sqdoc7.pdf

Gill P E, Murray W and Saunders M A (2005b) Users' guide for SNOPT 7.1: a Fortran package for large-scale linear nonlinear programming *Report NA 05-2* Department of Mathematics, University of California, San Diego http://www.ccom.ucsd.edu/~peg/papers/sndoc7.pdf

Gill P E, Murray W, Saunders M A and Wright M H (1986) Users' guide for NPSOL (Version 4.0): a Fortran package for nonlinear programming *Report SOL 86-2* Department of Operations Research, Stanford University

Gill P E, Murray W, Saunders M A and Wright M H (1992) Some theoretical properties of an augmented Lagrangian merit function *Advances in Optimization and Parallel Computing* (ed P M Pardalos) 101–128 North Holland

Gill P E, Murray W and Wright M H (1981) *Practical Optimization* Academic Press

Hock W and Schittkowski K (1981) *Test Examples for Nonlinear Programming Codes. Lecture Notes in Economics and Mathematical Systems* **187** Springer–Verlag

5 Arguments

1: **n** – Integer *Input*

On entry: n, the number of variables.

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

2: **nclin** – Integer *Input*

On entry: n_L, the number of general linear constraints.

Constraint: $\mathbf{nclin} \geq 0$.

3: **ncnln** – Integer *Input*

On entry: n_N, the number of nonlinear constraints.

Constraint: $\mathbf{ncnln} \geq 0$.

4: **tda** – Integer *Input*

On entry: the stride separating matrix column elements in the array **a**.

Constraints:

if **nclin** > 0, **tda** $\geq$ **n**;
otherwise **tda** ≥ 1.

5: **tdcj** – Integer *Input*

On entry: the stride separating matrix column elements in the array **cjac**.

Constraints:

if **ncnln** > 0, **tdcj** $\geq$ **n**;
otherwise **tdcj** ≥ 1.

6: **tdh** – Integer *Input*

On entry: the stride separating matrix column elements in the array **h**.

Constraint: **tdh** $\geq$ **n** unless the optional argument **Hessian Limited Memory** is in effect. If **Hessian Limited Memory** is in effect, array **h** is not referenced

7: **a**$[dim]$ – const double *Input*

Note: the dimension, *dim*, of the array **a** must be at least $\max(1, \textbf{nclin} \times \textbf{tda})$.

The (i, j)th element of the matrix A is stored in **a**$[(i-1) \times \textbf{tda} + j - 1]$.

On entry: the ith row of **a** contains the ith row of the matrix A_L of general linear constraints in (1). That is, the ith row contains the coefficients of the ith general linear constraint, for $i = 1, 2, \ldots,$ **nclin**.

If **nclin** $= 0$, the array **a** is not referenced.

8: **bl**$[\textbf{n} + \textbf{nclin} + \textbf{ncnln}]$ – const double *Input*
9: **bu**$[\textbf{n} + \textbf{nclin} + \textbf{ncnln}]$ – const double *Input*

On entry: **bl** must contain the lower bounds and **bu** the upper bounds for all the constraints, in the following order. The first n elements of each array must contain the bounds on the variables, the next n_L elements the bounds for the general linear constraints (if any) and the next n_N elements the bounds for the general nonlinear constraints (if any). To specify a nonexistent lower bound (i.e., $l_j = -\infty$), set **bl**$[j-1] \leq -bigbnd$, and to specify a nonexistent upper bound (i.e., $u_j = +\infty$), set **bu**$[j-1] \geq bigbnd$; where $bigbnd$ is the optional argument **Infinite Bound Size**. To specify the jth constraint as an *equality*, set **bl**$[j-1] =$ **bu**$[j-1] = \beta$, say, where $|\beta| < bigbnd$.

Constraints:

bl$[j-1] \leq$ **bu**$[j-1]$, for $j = 1, 2, \ldots,$ **n** + **nclin** + **ncnln**;
if **bl**$[j-1] =$ **bu**$[j-1] = \beta$, $|\beta| < bigbnd$.

10: **confun** – function, supplied by the user *External Function*

confun must calculate the vector $c(x)$ of nonlinear constraint functions and (optionally) its Jacobian, $\dfrac{\partial c}{\partial x}$, for a specified n-vector x. If there are no nonlinear constraints (i.e., **ncnln** $= 0$), nag_opt_nlp_solve (e04wdc) will never call **confun**, so it may be specified as NULLFN. If there are nonlinear constraints, the first call to **confun** will occur before the first call to **objfun**.

If all constraint gradients (Jacobian elements) are known (i.e., **Derivative Level** $= 2$ or 3), any *constant* elements may be assigned to **cjac** once only at the start of the optimization. An element of **cjac** that is not subsequently assigned in **confun** will retain its initial value throughout. Constant elements may be loaded in **cjac** during the first call to **confun** (signalled by the value of **nstate** $= 1$). The ability to preload constants is useful when many Jacobian elements are identically zero, in which case **cjac** may be initialized to zero and nonzero elements may be reset by **confun**.

It must be emphasized that, if **Derivative Level** < 2, unassigned elements of **cjac** are *not* treated as constant; they are estimated by finite differences, at nontrivial expense.

The specification of **confun** is:

```
void confun (Integer *mode, Integer ncnln, Integer n, Integer tdcj,
     const Integer needc[], const double x[], double ccon[],
     double cjac[], Integer nstate, Nag_Comm *comm)
```

1: **mode** – Integer * *Input/Output*

On entry: is set by nag_opt_nlp_solve (e04wdc) to indicate which values must be assigned during each call of **confun**. Only the following values need be assigned, for each value of i such that **needc**$[i-1] > 0$:

mode $= 0$
The components of **ccon** corresponding to positive values in **needc** must be set. Other components and the array **cjac** are ignored.

mode $= 1$
The known components of the rows of **cjac** corresponding to positive values in **needc** must be set. Other rows of **cjac** and the array **ccon** will be ignored.

mode $= 2$
Only the elements of **ccon** corresponding to positive values of **needc** need to be set (and similarly for the known components of the rows of **cjac**).

On exit: may be used to indicate that you are unable or unwilling to evaluate the constraint functions at the current x.

During the linesearch, the constraint functions are evaluated at points of the form $x = x_k + \alpha p_k$ after they have already been evaluated satisfactorily at x_k. At any such α, if you set **mode** $= -1$, nag_opt_nlp_solve (e04wdc) will evaluate the functions at some point closer to x_k (where they are more likely to be defined).

If for some reason you wish to terminate the current problem, set **mode** < -1.

2: **ncnln** – Integer *Input*

On entry: n_N, the number of nonlinear constraints.

3: **n** – Integer *Input*

On entry: n, the number of variables.

4: **tdcj** – Integer *Input*

On entry: the stride used in the array **cjac**.

5: **needc**[**ncnln**] – const Integer *Input*

On entry: the indices of the elements of **ccon** and/or **cjac** that must be evaluated by **confun**. If **needc**$[i-1] > 0$, the ith element of **ccon** and/or the available elements of the ith row of **cjac** (see argument **mode**) must be evaluated at x.

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

On entry: x, the vector of variables at which the constraint functions and/or the available elements of the constraint Jacobian are to be evaluated.

7: **ccon**[**max**(**1**, **ncnln**)] – double *Output*

On exit: if **needc**$[i-1] > 0$ and **mode** $= 0$ or 2, **ccon**$[i-1]$ must contain the value of the ith constraint at x. The remaining elements of **ccon**, corresponding to the non-positive elements of **needc**, are ignored.

8: **cjac**[**ncnln** × **tdcj**] – double *Input/Output*

On entry: the elements of **cjac** are set to special values that enable nag_opt_nlp_solve (e04wdc) to detect whether they are reset by **confun**.

On exit: if **needc**$[i-1] > 0$ and **mode** $= 1$ or 2, the ith row of **cjac** must contain the available elements of the vector ∇c_i given by

$$\nabla c_i = \left(\frac{\partial c_i}{\partial x_1}, \frac{\partial c_i}{\partial x_2}, \ldots, \frac{\partial c_i}{\partial x_n}\right)^{\mathrm{T}},$$

where $\dfrac{\partial c_i}{\partial x_j}$ is the partial derivative of the ith constraint with respect to the jth variable, evaluated at the point x. See also the argument **nstate**. The remaining rows of **cjac**, corresponding to non-positive elements of **needc**, are ignored.

If all elements of the constraint Jacobian are known (i.e., **Derivative Level** $= 2$ or 3), any constant elements may be assigned to **cjac** one time only at the start of the optimization. An element of **cjac** that is not subsequently assigned in **confun** will retain its initial value throughout. Constant elements may be loaded into **cjac** during the first call to **confun** (signalled by the value **nstate** $= 1$). The ability to preload constants is useful when many Jacobian elements are identically zero, in which case **cjac** may be initialized to zero and nonzero elements may be reset by **confun**.

Note that constant nonzero elements do affect the values of the constraints. Thus, if **cjac**$[(i-1) \times$ **tdcj** $+ j - 1]$ is set to a constant value, it need not be reset in subsequent calls to **confun**, but the value **cjac**$[(i-1) \times$ **tdcj** $+ j - 1] \times$ **x**$[j-1]$ must nonetheless be added to **ccon**$[i-1]$. For example, if **cjac**$[0] = 2$ and **cjac**$[1] = -5$ then the term $2 \times$ **x**$[0] - 5 \times$ **x**$[1]$ must be included in the definition of **ccon**$[0]$.

It must be emphasized that, if **Derivative Level** $= 0$ or 1, unassigned elements of **cjac** are not treated as constant; they are estimated by finite differences, at nontrivial expense. If you do not supply a value for the optional argument **Difference Interval**, an interval for each element of x is computed automatically at the start of the optimization. The automatic procedure can usually identify constant elements of **cjac**, which are then computed once only by finite differences.

9: **nstate** – Integer *Input*

On entry: if **nstate** $= 1$ then nag_opt_nlp_solve (e04wdc) is calling **confun** for the first time. This argument setting allows you to save computation time if certain data must be read or calculated only once.

10: **comm** – Nag_Comm *

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

user – double *
iuser – Integer *
p – Pointer

The type Pointer will be `void *`. Before calling nag_opt_nlp_solve (e04wdc) you may allocate memory and initialize these pointers with various quantities for use by **confun** when called from nag_opt_nlp_solve (e04wdc) (see Section 3.2.1.1 in the Essential Introduction).

confun should be tested separately before being used in conjunction with nag_opt_nlp_solve (e04wdc). See also the description of the optional argument **Verify Level**.

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

objfun must calculate the objective function $F(x)$ and (optionally) its gradient $g(x) = \dfrac{\partial F}{\partial x}$ for a specified n-vector x.

The specification of **objfun** is:

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

1: **mode** – Integer * *Input/Output*

On entry: is set by nag_opt_nlp_solve (e04wdc) to indicate which values must be assigned during each call of **objfun**. Only the following values need be assigned:

mode $= 0$
objf.

mode $= 1$
All available elements of **grad**.

mode $= 2$
objf and all available elements of **grad**.

On exit: may be used to indicate that you are unable or unwilling to evaluate the objective function at the current x.

During the linesearch, the function is evaluated at points of the form $x = x_k + \alpha p_k$ after they have already been evaluated satisfactorily at x_k. For any such x, if you set **mode** $= -1$, nag_opt_nlp_solve (e04wdc) will reduce α and evaluate the functions again (closer to x_k, where they are more likely to be defined).

If for some reason you wish to terminate the current problem, set **mode** < -1.

2: **n** – Integer *Input*

On entry: n, the number of variables.

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

On entry: x, the vector of variables at which the objective function and/or all available elements of its gradient are to be evaluated.

4: **objf** – double * *Output*

On exit: if **mode** $= 0$ or 2, **objf** must be set to the value of the objective function at x.

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

On entry: the elements of **grad** are set to special values.

On exit: if **mode** $= 1$ or 2, **grad** must return the available elements of the gradient evaluated at x, i.e., **grad**$[i-1]$ contains the partial derivative $\dfrac{\partial F}{\partial x_i}$.

6: **nstate** – Integer *Input*

On entry: if **nstate** $= 1$ then nag_opt_nlp_solve (e04wdc) is calling **objfun** for the first time. This argument setting allows you to save computation time if certain data must be read or calculated only once.

7: **comm** – Nag_Comm *

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

user – double *
iuser – Integer *
p – Pointer

The type Pointer will be `void *`. Before calling nag_opt_nlp_solve (e04wdc) you may allocate memory and initialize these pointers with various quantities for use by **objfun** when called from nag_opt_nlp_solve (e04wdc) (see Section 3.2.1.1 in the Essential Introduction).

objfun should be tested separately before being used in conjunction with nag_opt_nlp_solve (e04wdc). See also the description of the optional argument **Verify Level**.

12: **majits** – Integer * *Output*

On exit: the number of major iterations performed.

13: **istate**[**n** + **nclin** + **ncnln**] – Integer *Input/Output*

On entry: is an integer array that need not be initialized if nag_opt_nlp_solve (e04wdc) is called with the **Cold Start** option (the default).

If optional argument **Warm Start** has been chosen, every element of **istate** must be set. If nag_opt_nlp_solve (e04wdc) has just been called on a problem with the same dimensions, **istate** already contains valid values. Otherwise, **istate**$[j-1]$ should indicate whether either of the constraints $r_j(x) \geq l_j$ or $r_j(x) \leq u_j$ is expected to be active at a solution of (1).

The ordering of **istate** is the same as for **bl**, **bu** and $r(x)$, i.e., the first **n** components of **istate** refer to the upper and lower bounds on the variables, the next **nclin** refer to the bounds on $A_L x$, and the last **ncnln** refer to the bounds on $c(x)$. Possible values of **istate**$[i-1]$ follow:

0 Neither $r_j(x) \geq l_j$ nor $r_j(x) \leq u_j$ is expected to be active.
1 $r_j(x) \geq l_j$ is expected to be active.
2 $r_j(x) \leq u_j$ is expected to be active.
3 This may be used if $l_j = u_j$. Normally an equality constraint $r_j(x) = l_j = u_j$ is active at a solution.

The values 1, 2 or 3 all have the same effect when **bl**$[j-1] =$ **bu**$[j-1]$. If necessary, nag_opt_nlp_solve (e04wdc) will override your specification of **istate**, so that a poor choice will not cause the algorithm to fail.

On exit: describes the status of the constraints $l \leq r(x) \leq u$. For the jth lower or upper bound, $j = 1, 2, \ldots,$ **n** + **nclin** + **ncnln**, the possible values of **istate**$[j-1]$ are as follows (see Figure 1). δ is the appropriate feasibility tolerance.

-2 (Region 1) The lower bound is violated by more than δ.
-1 (Region 5) The upper bound is violated by more than δ.
0 (Region 3) Both bounds are satisfied by more than δ.
1 (Region 2) The lower bound is active (to within δ).
2 (Region 4) The upper bound is active (to within δ).
3 (Region 2 = Region 4) The bounds are equal and the equality constraint is satisfied (to within δ).

These values of **istate** are labelled in the printed solution according to Table 1.

Region	1	2	3	4	5	
$2 \equiv 4$						

istate$[j-1]$	-2	1	0	2	-1	3
Printed solution	--	LL	FR	UL	++	EQ

Table 1
Labels used in the printed solution for the regions in Figure 1

14: **ccon**[**max**(**1**, **ncnln**)] – double *Input/Output*

On entry: **ccon** need not be initialized if the (default) optional argument **Cold Start** is used.

For a **Warm Start**, and if **ncnln** > 0, **ccon** contains values of the nonlinear constraint functions c_i, for $i = 1, 2, \ldots,$ **ncnln**, calculated in a previous call to nag_opt_nlp_solve (e04wdc).

On exit: if **ncnln** > 0, **ccon**$[i-1]$ contains the value of the ith nonlinear constraint function c_i at the final iterate, for $i = 1, 2, \ldots,$ **ncnln**.

If **ncnln** $= 0$, the array **ccon** is not referenced.

15: **cjac**$[dim]$ – double *Input/Output*

Note: the dimension, *dim*, of the array **cjac** must be at least $\max(1,$ **ncnln** $\times$ **tdcj**$)$.

On entry: in general, **cjac** need not be initialized before the call to nag_opt_nlp_solve (e04wdc). However, if **Derivative Level** $= 2$ or 3, any constant elements of **cjac** may be initialized. Such elements need not be reassigned on subsequent calls to **confun**.

On exit: if **ncnln** > 0, **cjac** contains the Jacobian matrix of the nonlinear constraint functions at the final iterate, i.e., **cjac**$[(i-1) \times$ **tdcj** $+ j - 1]$ contains the partial derivative of the ith constraint function with respect to the jth variable, for $i = 1, 2, \ldots,$ **ncnln** and $j = 1, 2, \ldots,$ **n**. (See the discussion of argument **cjac** under **confun**.)

If **ncnln** $= 0$, the array **cjac** is not referenced.

16: **clamda**[**n** + **nclin** + **ncnln**] – double *Input/Output*

On entry: need not be set if the (default) optional argument **Cold Start** is used.

If the optional argument **Warm Start** has been chosen, **clamda**$[j-1]$ must contain a multiplier estimate for each nonlinear constraint, with a sign that matches the status of the constraint specified by the **istate** array, for $j =$ **n** + **nclin** $+ 1, \ldots,$ **n** + **nclin** + **ncnln**. The remaining elements need not be set. If the jth constraint is defined as 'inactive' by the initial value of the **istate** array (i.e., **istate**$[j-1] = 0$), **clamda**$[j-1]$ should be zero; if the jth constraint is an inequality active at its lower bound (i.e., **istate**$[j-1] = 1$), **clamda**$[j-1]$ should be non-negative; if the jth constraint is an inequality active at its upper bound (i.e., **istate**$[j-1] = 2$), **clamda**$[j-1]$ should be non-positive. If necessary, the function will modify **clamda** to match these rules.

On exit: the values of the QP multipliers from the last QP subproblem. **clamda**$[j-1]$ should be non-negative if **istate**$[j-1] = 1$ and non-positive if **istate**$[j-1] = 2$.

17: **objf** – double * *Output*

On exit: the value of the objective function at the final iterate.

18: **grad**[**n**] – double *Output*

On exit: the gradient of the objective function (or its finite difference approximation) at the final iterate.

19: **h**$[dim]$ – double *Input/Output*

Note: the dimension, *dim*, of the array **h** must be at least **n** $\times$ **tdh**.

On entry: **h** need not be initialized if the (default) optional argument **Cold Start** is used, and will be set to the identity.

If the optional argument **Warm Start** has been chosen, **h** provides the initial approximation of the Hessian of the Lagrangian, i.e., $\mathbf{h}[(i-1)\times\mathbf{tdh}+j-1]\approx\frac{\partial^2\mathcal{L}(x,\lambda)}{\partial x_i\partial x_j}$, where $\mathcal{L}(x,\lambda)=F(x)-c(x)^{\mathrm{T}}\lambda$ and λ is an estimate of the Lagrange multipliers. **h** must be a positive definite matrix.

On exit: contains the Hessian of the Lagrangian at the final estimate x.

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

On entry: an initial estimate of the solution.

On exit: the final estimate of the solution.

21: **state** – Nag_E04State * *Communication Structure*

state contains internal information required for functions in this suite. It must not be modified in any way.

22: **comm** – Nag_Comm *

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

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

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

nag_opt_nlp_solve (e04wdc) returns with **fail.code** = NE_NOERROR if the iterates have converged to a point x that satisfies the first-order Kuhn–Tucker (see Section 13.2) conditions to the accuracy requested by the **Major Optimality Tolerance**, i.e., the projected gradient and active constraint residuals are negligible at x.

You should check whether the following four conditions are satisfied:

(i) the final value of `rgNorm` (see Section 13.2) is significantly less than that at the starting point;

(ii) during the final major iterations, the values of `Step` and `Minors` (see Section 13.1) are both one;

(iii) the last few values of both `rgNorm` and `SumInf` (see Section 13.2) become small at a fast linear rate; and

(iv) `condHz` (see Section 13.1) is small.

If all these conditions hold, x is almost certainly a local minimum of (1).

One caution about 'Optimal solutions'. Some of the variables or slacks may lie outside their bounds more than desired, especially if scaling was requested. `Max Primal infeas` in the Print file refers to the largest bound infeasibility and which variable is involved. If it is too large, consider restarting with a smaller **Minor Feasibility Tolerance** (say 10 times smaller) and perhaps **Scale Option** = 0.

Similarly, `Max Dual infeas` in the Print file indicates which variable is most likely to be at a nonoptimal value. Broadly speaking, if

$$\texttt{Max Dual infeas}/\texttt{Max pi} = 10^{-d},$$

then the objective function would probably change in the dth significant digit if optimization could be continued. If d seems too large, consider restarting with a smaller **Major Optimality Tolerance**.

Finally, `Nonlinear constraint violn` in the Print file shows the maximum infeasibility for nonlinear rows. If it seems too large, consider restarting with a smaller **Major Feasibility Tolerance**.

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_ALLOC_INSUFFICIENT

Internal memory allocation was insufficient. Please contact NAG.

NE_BAD_PARAM

Basis file dimensions do not match this problem.

On entry, argument ⟨*value*⟩ had an illegal value.

NE_BASIS_FAILURE

An error has occurred in the basis package, perhaps indicating incorrect setup of arrays. Set the optional argument **Print File** and examine the output carefully for further information.

NE_DERIV_ERRORS

User-supplied function computes incorrect constraint derivatives.

User-supplied function computes incorrect objective derivatives.

If the message refers to the derivatives of the objective function, then a check has been made on some individual elements of the objective gradient array at the first point that satisfies the linear constraints. At least one component **grad**$j-1$ *is being set to a value that disagrees markedly with its associated forward-difference estimate* $\frac{\partial F}{\partial x_j}$*. (The relative difference between the computed and estimated values is 1.0 or more.) This exit is a safeguard, since nag_opt_nlp_solve (e04wdc) will usually fail to make progress when the computed gradients are seriously inaccurate. In the process it may expend considerable effort before terminating with* **fail**.**code** = *NE_NUM_DIFFICULTIES.*

Check the function and gradient computation very carefully in ***objfun****. A simple omission could explain everything. If* F *or a component* $\frac{\partial F}{\partial x_j}$ *is very large, then give serious thought to scaling the function or the nonlinear variables.*

If you feel certain that the computed **grad**$[j-1]$ *is correct (and that the forward-difference estimate is therefore wrong), you can specify* **Verify Level** = *0 to prevent individual elements from being checked. However, the optimization procedure may have difficulty.*

If the message refers to derivatives of the constraints, then at least one of the computed constraint derivatives is significantly different from an estimate obtained by forward-differencing the vector $c(x)$*. Follow the advice given above, trying to ensure that the arrays* ***ccon*** *and* ***cjac*** *are being set correctly in* ***confun****.*

NE_E04WCC_NOT_INIT

The initialization function nag_opt_nlp_init (e04wcc) has not been called.

NE_INT

On entry, **n** = ⟨*value*⟩.
Constraint: **n** > 0.

On entry, **nclin** = ⟨*value*⟩.
Constraint: **nclin** ≥ 0.

On entry, **ncnln** = ⟨*value*⟩.
Constraint: **ncnln** ≥ 0.

On entry, **tda** = ⟨*value*⟩.
Constraint: **tda** > 0.

On entry, **tdcj** $= \langle value \rangle$.
Constraint: **tdcj** > 0.

On entry, **tdh** $= \langle value \rangle$.
Constraint: **tdh** > 0.

NE_INT_2

On entry, **nclin** $= \langle value \rangle$ and **n** $= \langle value \rangle$.
Constraint: **n** > 0.

On entry, **ncnln** $= \langle value \rangle$ and **n** $= \langle value \rangle$.
Constraint: **n** > 0.

On entry, **tda** $= \langle value \rangle$ and **nclin** $= \langle value \rangle$.
Constraint: **tda** $\geq$ **nclin**.

On entry, **tdcj** $= \langle value \rangle$ and **ncnln** $= \langle value \rangle$.
Constraint: **tdcj** $\geq$ **ncnln**.

On entry, **tdh** $= \langle value \rangle$ and **n** $= \langle value \rangle$.
Constraint: **tdh** $\geq$ **n**.

NE_INT_3

On entry, **tda** $= \langle value \rangle$, **nclin** $= \langle value \rangle$ and **n** $= \langle value \rangle$.
Constraint: if **nclin** > 0, **tda** $\geq$ **n**;
otherwise **tda** ≥ 1.

On entry, **tdcj** $= \langle value \rangle$, **ncnln** $= \langle value \rangle$ and **n** $= \langle value \rangle$.
Constraint: if **ncnln** > 0, **tdcj** $\geq$ **n**;
otherwise **tdcj** ≥ 1.

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.

An unexpected error has occurred. Set the optional argument **Print File** and examine the output carefully for further information.

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_NOT_REQUIRED_ACC

The requested accuracy could not be achieved.

A feasible solution has been found, but the requested accuracy in the dual infeasibilities could not be achieved. An abnormal termination has occurred, but nag_opt_nlp_solve (e04wdc) is within 10^{-2} of satisfying the **Major Optimality Tolerance**. *Check that the* **Major Optimality Tolerance** *is not too small.*

NE_NUM_DIFFICULTIES

Numerical difficulties have been encountered and no further progress can be made.

Numerical difficulties have been encountered and no further progress can be made.

Several circumstances could lead to this exit.

1. The user-supplied functions **objfun** or **confun** could be returning accurate function values but inaccurate gradients (or vice versa). This is the most likely cause. Study the comments given for **fail**.**code** = NE_DERIV_ERRORS, and do your best to ensure that the coding is correct.
2. The function and gradient values could be consistent, but their precision could be too low. For example, accidental use of a real data type when double precision was intended would lead to a relative function precision of about 10^{-6} instead of something like 10^{-15}. The default **Major Optimality Tolerance** of 2×10^{-6} would need to be raised to about 10^{-3} for optimality to be declared (at a rather suboptimal point). Of course, it is better to revise the function coding to obtain as much precision as economically possible.
3. If function values are obtained from an expensive iterative process, they may be accurate to rather few significant figures, and gradients will probably not be available. One should specify

   Function Precision t

   Major Optimality Tolerance $\sqrt{t}$

   but even then, if t is as large as 10^{-5} or 10^{-6} (only 5 or 6 significant figures), the same exit condition may occur. At present the only remedy is to increase the accuracy of the function calculation.
4. An LU factorization of the basis has just been obtained and used to recompute the basic variables x_B, given the present values of the superbasic and nonbasic variables. A step of 'iterative refinement' has also been applied to increase the accuracy of x_B. However, a row check has revealed that the resulting solution does not satisfy the current constraints $Ax - s = 0$ sufficiently well.

   This probably means that the current basis is very ill-conditioned. If there are some linear constraints and variables, try **Scale Option** = 1 if scaling has not yet been used.

   For certain highly structured basis matrices (notably those with band structure), a systematic growth may occur in the factor U. Consult the description of `Umax` and `Growth` in Section 13.4 and set the **LU Factor Tolerance** to 2.0 (or possibly even smaller, but not less than 1.0).
5. The first factorization attempt will have found the basis to be structurally or numerically singular. (Some diagonals of the triangular matrix U were respectively zero or smaller than a certain tolerance.) The associated variables are replaced by slacks and the modified basis is refactorized, but singularity persists. This must mean that the problem is badly scaled, or the **LU Factor Tolerance** is too much larger than 1.0. This is highly unlikely to occur.

NE_REAL_2

On entry, bounds **bl** and **bu** for ⟨*value*⟩ are equal and infinite. **bl** = **bu** = ⟨*value*⟩ and $bigbnd = \langle value \rangle$.

On entry, bounds for ⟨*value*⟩ are inconsistent. **bl** = ⟨*value*⟩ and **bu** = ⟨*value*⟩.

NE_UNBOUNDED

The problem appears to be unbounded. The constraint violation limit has been reached.

The problem appears to be unbounded. The objective function is unbounded.

The problem appears to be unbounded (or badly scaled).

For linear problems, unboundedness is detected by the simplex method when a nonbasic variable can be increased or decreased by an arbitrary amount without causing a basic variable to violate a bound. Consider adding an upper or lower bound to the variable. Also, examine the constraints that have nonzeros in the associated column, to see if they have been formulated as intended.

Very rarely, the scaling of the problem could be so poor that numerical error will give an erroneous indication of unboundedness. Consider using the optional argument **Scale Option**.

For nonlinear problems, nag_opt_nlp_solve (e04wdc) monitors both the size of the current objective function and the size of the change in the variables at each step. If either of these is very large (as judged by the unbounded arguments (see Section 13.1)), the problem is terminated and declared unbounded. To avoid large function values, it may be necessary to impose bounds on some of the variables in order to keep them away from singularities in the nonlinear functions.

The message may indicate an abnormal termination while enforcing the limit on the constraint violations. This exit implies that the objective is not bounded below in the feasible region defined by expanding the bounds by the value of the **Violation Limit**.

NE_USER_STOP

User-supplied constraint function requested termination.

User-supplied objective function requested termination.

You have indicated the wish to terminate solution of the current problem by setting ***mode*** *to a value* < -1 *on exit from* ***objfun*** *or* ***confun***.

NE_USRFUN_UNDEFINED

Unable to proceed into undefined region of user-supplied function.

User-supplied function is undefined at the first feasible point.

User-supplied function is undefined at the initial point.

You have indicated that the problem functions are undefined by assigning the value **mode** $= -1$ *on exit from* ***objfun*** *or* ***confun***. *nag_opt_nlp_solve (e04wdc) attempts to evaluate the problem functions closer to a point at which the functions are already known to be defined. This exit occurs if nag_opt_nlp_solve (e04wdc) is unable to find a point at which the functions are defined. This will occur in the case of:*

– undefined functions with no recovery possible;

– undefined functions at the first point;

– undefined functions at the first feasible point; or

– undefined functions when checking derivatives.

NW_LIMIT_REACHED

Iteration limit reached.

Major iteration limit reached.

The value of the optional argument **Superbasics Limit** is too small.

Either the **Iterations Limit** *or the* **Major Iterations Limit** *was exceeded before the required solution could be found. Check the iteration log to be sure that progress was being made. If so, and if you caused a basis file to be saved by using the optional argument* **New Basis File**, *consider restarting the run using the optional argument* **Old Basis File** *to see whether further progress can be made. If you have no basis file available, you might rerun the problem after increasing the optional arguments* **Minor Iterations Limit** *and/or* **Major Iterations Limit**

If none of the above limits have been reached, this error may mean that the problem appears to be more nonlinear than anticipated. The current set of basic and superbasic variables have been optimized as much as possible and a pricing operation (where a nonbasic variable is selected to become superbasic) is necessary to continue, but it can't continue as the number of superbasic variables has already reached the limit specified by the optional argument **Superbasics Limit**. *In general, raise the* **Superbasics Limit** s *by a reasonable amount, bearing in mind the storage needed for the reduced Hessian. (The* **Reduced Hessian Dimension** h *will also increase to* s *unless specified otherwise, and the associated storage will be about* $\frac{1}{2}s^2$ *words.) In some cases you may have to set* $h < s$ *to conserve storage, but beware that the rate of convergence will probably fall off severely.*

NW_NOT_FEASIBLE

The linear constraints appear to be infeasible.

The problem appears to be infeasible. Infeasibilites have been minimized.

The problem appears to be infeasible. Nonlinear infeasibilites have been minimized.

The problem appears to be infeasible. The linear equality constraints could not be satisfied.

When the constraints are linear, this message is based on a relatively reliable indicator of infeasibility. Feasibility is measured with respect to the upper and lower bounds on the variables and slacks. Among all the points satisfying the general constraints $Ax - s = 0$ (see (5) and (6) in Section 11.2), there is apparently no point that satisfies the bounds on x and s. Violations as small as the **Minor Feasibility Tolerance** *are ignored, but at least one component of x or s violates a bound by more than the tolerance.*

When nonlinear constraints are present, infeasibility is much harder to recognize correctly. Even if a feasible solution exists, the current linearization of the constraints may not contain a feasible point. In an attempt to deal with this situation, when solving each QP subproblem, nag_opt_nlp_solve (e04wdc) is prepared to relax the bounds on the slacks associated with nonlinear rows.

If a QP subproblem proves to be infeasible or unbounded (or if the Lagrange multiplier estimates for the nonlinear constraints become large), nag_opt_nlp_solve (e04wdc) enters so-called 'nonlinear elastic' mode. The subproblem includes the original QP objective and the sum of the infeasibilities – suitably weighted using the optional argument **Elastic Weight**. *In elastic mode, some of the bounds on the nonlinear rows are 'elastic' – i.e., they are allowed to violate their specific bounds. Variables subject to elastic bounds are known as elastic variables. An elastic variable is free to violate one or both of its original upper or lower bounds. If the original problem has a feasible solution and the elastic weight is sufficiently large, a feasible point eventually will be obtained for the perturbed constraints, and optimization can continue on the subproblem. If the nonlinear problem has no feasible solution, nag_opt_nlp_solve (e04wdc) will tend to determine a 'good' infeasible point if the elastic weight is sufficiently large. (If the elastic weight were infinite, nag_opt_nlp_solve (e04wdc) would locally minimize the nonlinear constraint violations subject to the linear constraints and bounds.)*

Unfortunately, even though nag_opt_nlp_solve (e04wdc) locally minimizes the nonlinear constraint violations, there may still exist other regions in which the nonlinear constraints are satisfied. Wherever possible, nonlinear constraints should be defined in such a way that feasible points are known to exist when the constraints are linearized.

7 Accuracy

If **fail**.**code** = NE_NOERROR on exit, then the vector returned in the array **x** is an estimate of the solution to an accuracy of approximately **Major Optimality Tolerance**.

8 Parallelism and Performance

nag_opt_nlp_solve (e04wdc) is not threaded by NAG in any implementation.

nag_opt_nlp_solve (e04wdc) makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this function. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 Further Comments

This section describes the final output produced by nag_opt_nlp_solve (e04wdc). Intermediate and other output are given in Section 13.

9.1 The Final Output

If **Print File** $= 0$, the final output, including a listing of the status of every variable and constraint will be sent to the **Print File**. The following describes the output for each variable. A full stop (.) is printed for any numerical value that is zero.

`Variable` gives the name (`Variable`) and index j, for $j = 1, 2, \ldots, n$, of the variable.

`State` gives the state of the variable (`FR` if neither bound is in the working set, `EQ` if a fixed variable, `LL` if on its lower bound, `UL` if on its upper bound, `TF` if temporarily fixed at its current value). If `Value` lies outside the upper or lower bounds by more than the **Feasibility Tolerance**, `State` will be `++` or `--` respectively. (The latter situation can occur only when there is no feasible point for the bounds and linear constraints.)

A key is sometimes printed before `State`.

- `A` *Alternative optimum possible*. The variable is active at one of its bounds, but its Lagrange multiplier is essentially zero. This means that if the variable were allowed to start moving away from its bound then there would be no change to the objective function. The values of the other free variables *might* change, giving a genuine alternative solution. However, if there are any degenerate variables (labelled `D`), the actual change might prove to be zero, since one of them could encounter a bound immediately. In either case the values of the Lagrange multipliers might also change.
- `D` *Degenerate*. The variable is free, but it is equal to (or very close to) one of its bounds.
- `I` *Infeasible*. The variable is currently violating one of its bounds by more than the **Feasibility Tolerance**.

`Value` is the value of the variable at the final iteration.

`Lower bound` is the lower bound specified for the variable. `None` indicates that $\mathbf{bl}[j-1] \leq -bigbnd$.

`Upper bound` is the upper bound specified for the variable. `None` indicates that $\mathbf{bu}[j-1] \geq bigbnd$.

`Lagr multiplier` is the Lagrange multiplier for the associated bound. This will be zero if `State` is `FR` unless $\mathbf{bl}[j-1] \leq -bigbnd$ and $\mathbf{bu}[j-1] \geq bigbnd$, in which case the entry will be blank. If x is optimal, the multiplier should be non-negative if `State` is `LL` and non-positive if `State` is `UL`.

`Slack` is the difference between the variable `Value` and the nearer of its (finite) bounds $\mathbf{bl}[j-1]$ and $\mathbf{bu}[j-1]$. A blank entry indicates that the associated variable is not bounded (i.e., $\mathbf{bl}[j-1] \leq -bigbnd$ and $\mathbf{bu}[j-1] \geq bigbnd$).

The meaning of the output for linear and nonlinear constraints is the same as that given above for variables, with $\mathbf{bl}[j-1]$ and $\mathbf{bu}[j-1]$ replaced by $\mathbf{bl}[n+j-1]$ and $\mathbf{bu}[n+j-1]$ respectively, and with the following changes in the heading:

`Linear constrnt` gives the name (`lincon`) and index j, for $j = 1, 2, \ldots, n_L$, of the linear constraint.

`Nonlin constrnt` gives the name (`nlncon`) and index $(j - n_L)$, for $j = n_L + 1, \ldots, n_L + n_N$, of the nonlinear constraint.

Note that movement off a constraint (as opposed to a variable moving away from its bound) can be interpreted as allowing the entry in the `Slack` column to become positive.

Numerical values are output with a fixed number of digits; they are not guaranteed to be accurate to this precision.

10 Example

This example is based on Problem 71 in Hock and Schittkowski (1981) and involves the minimization of the nonlinear function

$$F(x) = x_1x_4(x_1 + x_2 + x_3) + x_3$$

subject to the bounds

$$\begin{gathered} 1 \leq x_1 \leq 5 \\ 1 \leq x_2 \leq 5 \\ 1 \leq x_3 \leq 5 \\ 1 \leq x_4 \leq 5, \end{gathered}$$

to the general linear constraint

$$x_1 + x_2 + x_3 + x_4 \leq 20,$$

and to the nonlinear constraints

$$\begin{gathered} x_1^2 + x_2^2 + x_3^2 + x_4^2 \leq 40, \\ x_1x_2x_3x_4 \geq 25. \end{gathered}$$

The initial point, which is infeasible, is

$$x_0 = (1, 5, 5, 1)^{\mathrm{T}},$$

with $F(x_0) = 16$.

The optimal solution (to five figures) is

$$x^* = (1.0, 4.7430, 3.8211, 1.3794)^{\mathrm{T}},$$

and $F(x^*) = 17.014$. One bound constraint and both nonlinear constraints are active at the solution.

10.1 Program Text

```
/* nag_opt_nlp_solve (e04wdc) Example Program.
 *
 * Copyright 2014 Numerical Algorithms Group.
 *
 * Mark 8, 2004.
 */
#include <stdio.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nage04.h>

#ifdef __cplusplus
extern "C" {
#endif
static void NAG_CALL confun(Integer *mode, Integer ncnln, Integer n,
                            Integer ldcj, const Integer needc[],
                            const double x[], double ccon[], double cjac[],
                            Integer nstate, Nag_Comm *comm);
static void NAG_CALL objfun(Integer *mode, Integer n, const double x[],
                            double *objf, double grad[], Integer nstate,
                            Nag_Comm *comm);
#ifdef __cplusplus
}
#endif

int main(void)
{

  /* Scalars */
  double       objf;
  Integer      exit_status, i, j, majits, n, nclin, ncnln, nctotal, pda, pdcj,
               pdh;
```

```
  /* Arrays */
  static double ruser[2] = {-1.0, -1.0};
  double       *a = 0, *bl = 0, *bu = 0, *ccon = 0, *cjac = 0, *clamda = 0;
  double       *grad = 0, *h = 0, *x = 0;
  Integer      *istate = 0;

  /* Nag Types */
  Nag_E04State state;
  NagError     fail;
  Nag_Comm     comm;
  Nag_FileID   fileid;

#define A(I, J) a[(I-1)*pda + J - 1]

  exit_status = 0;
  INIT_FAIL(fail);

  printf("nag_opt_nlp_solve (e04wdc) Example Program Results\n");

  /* For communication with user-supplied functions: */
  comm.user = ruser;

  /* Skip heading in data file */
#ifdef _WIN32
  scanf_s("%*[^\n] ");
#else
  scanf("%*[^\n] ");
#endif

#ifdef _WIN32
  scanf_s("%"NAG_IFMT"%"NAG_IFMT"%"NAG_IFMT"%*[^\n] ", &n, &nclin, &ncnln);
#else
  scanf("%"NAG_IFMT"%"NAG_IFMT"%"NAG_IFMT"%*[^\n] ", &n, &nclin, &ncnln);
#endif
  if (n > 0 && nclin >= 0 && ncnln >= 0)
    {
      /* Allocate memory */
      nctotal = n + nclin + ncnln;
      if (!(a = NAG_ALLOC(nclin*n, double)) ||
          !(bl = NAG_ALLOC(nctotal, double)) ||
          !(bu = NAG_ALLOC(nctotal, double)) ||
          !(ccon = NAG_ALLOC(ncnln, double)) ||
          !(cjac = NAG_ALLOC(ncnln*n, double)) ||
          !(clamda = NAG_ALLOC(nctotal, double)) ||
          !(grad = NAG_ALLOC(n, double)) ||
          !(h = NAG_ALLOC(n*n, double)) ||
          !(x = NAG_ALLOC(n, double)) ||
          !(istate = NAG_ALLOC(nctotal, Integer)))
        {
          printf("Allocation failure\n");
          exit_status = -1;
          goto END;
        }
      pda = n;
      pdcj = n;
      pdh = n;

      /* Read a, bl, bu and x from data file */
      if (nclin > 0)
        {
          for (i = 1; i <= nclin; ++i)
            {
              for (j = 1; j <= n; ++j)
                {
#ifdef _WIN32
                  scanf_s("%lf", &A(i, j));
#else
                  scanf("%lf", &A(i, j));
#endif
                }
            }
```

```
#ifdef _WIN32
          scanf_s("%*[^\n] ");
#else
          scanf("%*[^\n] ");
#endif
        }

      for (i = 1; i <= n+nclin+ncnln; ++i)
        {
#ifdef _WIN32
          scanf_s("%lf", &bl[i - 1]);
#else
          scanf("%lf", &bl[i - 1]);
#endif
        }
#ifdef _WIN32
      scanf_s("%*[^\n] ");
#else
      scanf("%*[^\n] ");
#endif

      for (i = 1; i <= n+nclin+ncnln; ++i)
        {
#ifdef _WIN32
          scanf_s("%lf", &bu[i - 1]);
#else
          scanf("%lf", &bu[i - 1]);
#endif
        }
#ifdef _WIN32
      scanf_s("%*[^\n] ");
#else
      scanf("%*[^\n] ");
#endif

      for (i = 1; i <= n; ++i)
        {
#ifdef _WIN32
          scanf_s("%lf", &x[i - 1]);
#else
          scanf("%lf", &x[i - 1]);
#endif
        }
#ifdef _WIN32
      scanf_s("%*[^\n] ");
#else
      scanf("%*[^\n] ");
#endif

      /* nag_opt_nlp_init (e04wcc).
       * Initialization function for nag_opt_nlp_solve (e04wdc)
       */
      nag_opt_nlp_init(&state, &fail);
      if (fail.code != NE_NOERROR)
        {
          printf("Initialisation of nag_opt_nlp_init (e04wcc) failed.\n%s\n",
                 fail.message);
          exit_status = 1;
          goto END;
        }

      /* By default nag_opt_nlp_solve (e04wdc) does not print monitoring
       * information. Call nag_open_file (x04acc) to set the print file fileid.
       */
      /* nag_open_file (x04acc).
       * Open unit number for reading, writing or appending, and
       * associate unit with named file
       */
      nag_open_file("", 2, &fileid, &fail);
      if (fail.code != NE_NOERROR)
        {
```

```
          exit_status = 2;
          goto END;
        }
      /* nag_opt_nlp_option_set_integer (e04wgc).
       * Set a single option for nag_opt_nlp_solve (e04wdc) from
       * an integer argument
       */
      fflush(stdout);
      nag_opt_nlp_option_set_integer("Print file", fileid, &state, &fail);

      /* Solve the problem. */
      /* nag_opt_nlp_solve (e04wdc).
       * Solves the nonlinear programming (NP) problem
       */
      nag_opt_nlp_solve(n, nclin, ncnln, pda, pdcj, pdh, a, bl, bu,
                        confun, objfun, &majits, istate, ccon, cjac, clamda,
                        &objf, grad, h, x, &state, &comm, &fail);
      fflush(stdout);

      if (fail.code == NE_NOERROR)
        {
          printf("\n\nFinal objective value = %11.3f\n", objf);

          printf("Optimal X = ");

          for (i = 1; i <= n; ++i)
            printf("%9.2f%s", x[i - 1], i%7 == 0 || i == n?"\n":" ");
        }
      else
        {
          printf(
                  "Error message from nag_opt_nlp_solve (e04wdc).\n%s\n",
                  fail.message);
          exit_status = 1;
          goto END;
        }

      if (fail.code != NE_NOERROR)
        exit_status = 2;

    }
 END:
  NAG_FREE(a);
  NAG_FREE(bl);
  NAG_FREE(bu);
  NAG_FREE(ccon);
  NAG_FREE(cjac);
  NAG_FREE(clamda);
  NAG_FREE(grad);
  NAG_FREE(h);
  NAG_FREE(x);
  NAG_FREE(istate);


  return exit_status;
}

#undef A


static void NAG_CALL objfun(Integer *mode, Integer n, const double x[],
                            double *objf, double grad[], Integer nstate,
                            Nag_Comm *comm)
{
  /* Routine to evaluate objective function and its 1st derivatives. */

  /* Function Body */
  if (comm->user[0] == -1.0)
    {
      fflush(stdout);
      printf("(User-supplied callback objfun, first invocation.)\n");
```

```
      comm->user[0] = 0.0;
      fflush(stdout);
    }
  if (*mode == 0 || *mode == 2)
    {
      *objf = x[0] * x[3] * (x[0] + x[1] + x[2]) + x[2];
    }

  if (*mode == 1 || *mode == 2)
    {
      grad[0] = x[3] * (x[0] * 2. + x[1] + x[2]);
      grad[1] = x[0] * x[3];
      grad[2] = x[0] * x[3] + 1.;
      grad[3] = x[0] * (x[0] + x[1] + x[2]);
    }

  return;
} /* objfun */


static void NAG_CALL confun(Integer *mode, Integer ncnln, Integer n,
                            Integer pdcj, const Integer needc[],
                            const double x[],
                            double ccon[], double cjac[], Integer nstate,
                            Nag_Comm *comm)
{
  /* Scalars */
  Integer i, j;

#define CJAC(I, J) cjac[(I-1)*pdcj + J-1]

  /* Routine to evaluate the nonlinear constraints and their 1st */
  /* derivatives. */


  /* Function Body */
  if (comm->user[1] == -1.0)
    {
      fflush(stdout);
      printf("(User-supplied callback confun, first invocation.)\n");
      comm->user[1] = 0.0;
      fflush(stdout);
    }
  if (nstate == 1)
    {
      /* First call to confun.  Set all Jacobian elements to zero. */
      /* Note that this will only work when 'Derivative Level = 3' */
      /* (the default; see Section 11.2). */
      for (j = 1; j <= n; ++j)
        {
          for (i = 1; i <= ncnln; ++i)
            {
              CJAC(i, j) = 0.;
            }
        }
    }

  if (needc[0] > 0)
    {
      if (*mode == 0 || *mode == 2)
        {
          ccon[0] = x[0] * x[0] + x[1] * x[1] + x[2] * x[2] + x[3] * x[3];
        }
      if (*mode == 1 || *mode == 2)
        {
          CJAC(1, 1) = x[0] * 2.;
          CJAC(1, 2) = x[1] * 2.;
          CJAC(1, 3) = x[2] * 2.;
          CJAC(1, 4) = x[3] * 2.;
        }
    }
```

```
  if (needc[1] > 0)
    {
      if (*mode == 0 || *mode == 2)
        {
          ccon[1] = x[0] * x[1] * x[2] * x[3];
        }
      if (*mode == 1 || *mode == 2)
        {
          CJAC(2, 1) = x[1] * x[2] * x[3];
          CJAC(2, 2) = x[0] * x[2] * x[3];
          CJAC(2, 3) = x[0] * x[1] * x[3];
          CJAC(2, 4) = x[0] * x[1] * x[2];
        }
    }

  return;
} /* confun */

#undef CJAC
```

10.2 Program Data

```
nag_opt_nlp_solve (e04wdc) Example Program Data
  4   1   2                                                  : N, NCLIN and NCNLN
  1.0   1.0   1.0   1.0                                      : Matrix A
  1.0   1.0   1.0   1.0  -1.0E+25  -1.0E+25  25.0           : Lower bounds BL
  5.0   5.0   5.0   5.0  20.0      40.0      1.0E+25        : Upper bounds BU
  1.0   5.0   5.0   1.0                                      : Initial vector X
```

10.3 Program Results

```
nag_opt_nlp_solve (e04wdc) Example Program Results

 Parameters
 ==========

 Files
 -----
 Solution file..........        0      Old basis file ........        0      (Print file)...........        6
 Insert file............        0      New basis file ........        0      (Summary file).........        0
 Punch file.............        0      Backup basis file......        0
 Load file..............        0      Dump file..............        0

 Frequencies
 -----------
 Print frequency........      100      Check frequency........       60      Save new basis map.....      100
 Summary frequency......      100      Factorization frequency       50      Expand frequency.......    10000

 QP subproblems
 --------------
 QPsolver Cholesky......
 Scale tolerance........    0.900      Minor feasibility tol..  1.00E-06      Iteration limit........    10000
 Scale option...........        0      Minor optimality  tol..  1.00E-06      Minor print level......        1
 Crash tolerance........    0.100      Pivot tolerance........  2.04E-11      Partial price..........        1
 Crash option...........        3      Elastic weight.........  1.00E+04      Prtl price section ( A)        4
                                       New superbasics........       99      Prtl price section (-I)        3

 The SQP Method
 --------------
 Minimize...............               Cold start.............                Proximal Point method..        1
 Nonlinear objectiv vars        4      Major optimality tol...  2.00E-06      Function precision.....  1.72E-13
 Unbounded step size....  1.00E+20      Superbasics limit......        4      Difference interval....  4.15E-07
 Unbounded objective....  1.00E+15      Reduced Hessian dim....        4      Central difference int.  5.57E-05
 Major step limit.......  2.00E+00      Derivative linesearch..               Derivative level.......        3
 Major iterations limit.      1000      Linesearch tolerance...   0.90000      Verify level...........        0
 Minor iterations limit.       500      Penalty parameter......  0.00E+00      Major Print Level......        1
```

```
 Hessian Approximation
 ---------------------
 Full-Memory Hessian....                Hessian updates........  99999999       Hessian frequency......  99999999
                                                                                Hessian flush..........  99999999

 Nonlinear constraints
 ---------------------
 Nonlinear constraints..         2      Major feasibility tol..  1.00E-06       Violation limit........  1.00E+06
 Nonlinear Jacobian vars         4

 Miscellaneous
 -------------
 LU factor tolerance....      1.10      LU singularity tol.....  2.04E-11       Timing level...........         0
 LU update tolerance....      1.10      LU swap tolerance......  1.03E-04       Debug level............         0
 LU partial  pivoting...                eps (machine precision)  1.11E-16       System information.....        No



 Matrix statistics
 -----------------
               Total      Normal        Free       Fixed     Bounded
 Rows              3           3           0           0           0
 Columns           4           0           0           0           4

 No. of matrix elements                  12     Density     100.000
 Biggest                          1.0000E+00  (excluding fixed columns,
 Smallest                         0.0000E+00   free rows, and RHS)

 No. of objective coefficients             0

 Nonlinear constraints       2     Linear constraints       1
 Nonlinear variables         4     Linear variables         0
 Jacobian  variables         4     Objective variables      4
 Total constraints           3     Total variables          4



(User-supplied callback confun, first invocation.)
(User-supplied callback objfun, first invocation.)
 The user has defined       8   out of       8   constraint gradients.
 The user has defined       4   out of       4   objective  gradients.

 Cheap test of user-supplied problem derivatives...

 The constraint gradients seem to be OK.

 -->  The largest discrepancy was    1.84E-07  in constraint     6


 The objective  gradients seem to be OK.

 Gradient projected in one direction   4.99993000077E+00
 Difference approximation              4.99993303560E+00



   Itns Major Minors    Step   nCon  Feasible   Optimal  MeritFunction     L+U BSwap     nS  condHz Penalty
      2     0      2             1   1.7E+00   2.8E+00  1.6000000E+01       7            2 1.0E+00         _  r
      4     1      2 1.0E+00      2   1.3E-01   3.2E-01  1.7726188E+01       8            1 6.2E+00 8.3E-02 _n r
      5     2      1 1.0E+00      3   3.7E-02   1.7E-01  1.7099571E+01       7            1 2.0E+00 8.3E-02 _s
      6     3      1 1.0E+00      4   2.2E-02   1.1E-02  1.7014005E+01       7            1 1.8E+00 8.3E-02 _
      7     4      1 1.0E+00      5   1.5E-04   6.0E-04  1.7014018E+01       7            1 1.8E+00 9.2E-02 _
      8     5      1 1.0E+00      6 ( 3.3E-07)  2.3E-05  1.7014017E+01       7            1 1.9E+00 3.6E-01 _
      9     6      1 1.0E+00      7 ( 4.2E-10)( 2.4E-08) 1.7014017E+01       7            1 1.9E+00 3.6E-01 _

 E04WDM EXIT   0 -- finished successfully
 E04WDM INFO   1 -- optimality conditions satisfied

 Problem name                     NLP
 No. of iterations                  9   Objective value      1.7014017287E+01
```

```
 No. of major iterations             6   Linear objective     0.0000000000E+00
 Penalty parameter           3.599E-01   Nonlinear objective  1.7014017287E+01
 No. of calls to funobj              8   No. of calls to funcon              8
 No. of superbasics                  1   No. of basic nonlinears             2
 No. of degenerate steps             0   Percentage                       0.00
 Max x                       2 4.7E+00   Max pi                      2 5.5E-01
 Max Primal infeas           0 0.0E+00   Max Dual infeas             3 4.8E-08
 Nonlinear constraint violn    2.7E-09


 Variable          State      Value       Lower bound     Upper bound   Lagr multiplier       Slack

 variable      1     LL    1.000000        1.000000        5.000000        1.087871           .
 variable      2     FR    4.743000        1.000000        5.000000            .           0.2570
 variable      3     FR    3.821150        1.000000        5.000000            .            1.179
 variable      4     FR    1.379408        1.000000        5.000000            .           0.3794


 Linear constrnt   State      Value       Lower bound     Upper bound   Lagr multiplier       Slack

 lincon        1     FR    10.94356          None          20.00000            .            9.056


 Nonlin constrnt   State      Value       Lower bound     Upper bound   Lagr multiplier       Slack

 nlncon        1     UL    40.00000          None          40.00000      -0.1614686        -0.2700E-08
 nlncon        2     LL    25.00000        25.00000          None         0.5522937        -0.2215E-08


Final objective value =      17.014
Optimal X =      1.00      4.74      3.82      1.38
```

Note: *the remainder of this document is intended for more advanced users. Section 11 contains a detailed description of the algorithm which may be needed in order to understand Sections 12 and 13. Section 12 describes the optional arguments which may be set by calls to nag_opt_nlp_option_set_string (e04wfc), nag_opt_nlp_option_set_integer (e04wgc) and/or nag_opt_nlp_option_set_double (e04whc). Section 13 describes the quantities which can be requested to monitor the course of the computation.*

11 Algorithmic Details

Here we summarise the main features of the SQP algorithm used in nag_opt_nlp_solve (e04wdc) and introduce some terminology used in the description of the function and its arguments. The SQP algorithm is fully described in Gill *et al.* (2002).

11.1 Constraints and Slack Variables

The upper and lower bounds on the $n_L + n_N$ components of $\begin{pmatrix} A_L x \\ c(x) \end{pmatrix}$ are said to define the *general constraints* of the problem. nag_opt_nlp_solve (e04wdc) converts the general constraints to equalities by introducing a set of *slack variables* $s = (s_1, s_2, \ldots, s_{n_L+n_N})^{\mathrm{T}}$. For example, the linear constraint $5 \leq 2x_1 + 3x_2 \leq \infty$ is replaced by $2x_1 + 3x_2 - s_1 = 0$ together with the bounded slack $5 \leq s_1 \leq \infty$. The minimization problem (1) can therefore be written in the equivalent form

$$\underset{x,s}{\text{minimize}} F(x) \quad \text{subject to} \quad \begin{pmatrix} A_L x \\ c(x) \end{pmatrix} - s = 0, \quad l \leq \begin{pmatrix} x \\ s \end{pmatrix} \leq u. \tag{2}$$

The general constraints become the equalities $A_L x - s_L = 0$ and $c(x) - s_N = 0$, where s_L and s_N are the *linear* and *nonlinear* slacks.

11.2 Major Iterations

The basic structure of the SQP algorithm involves *major* and *minor* iterations. The major iterations generate a sequence of iterates $\{x_k\}$ that satisfy the linear constraints and converge to a point that satisfies the nonlinear constraints and the first-order conditions for optimality. At each iterate x_k a QP

subproblem is used to generate a search direction towards the next iterate x_{k+1}. The constraints of the subproblem are formed from the linear constraints $A_L x - s_L = 0$ and the linearized constraint

$$c(x_k) + c'(x_k)(x - x_k) - s_N = 0, \tag{3}$$

where $c'(x_k)$ denotes the *Jacobian matrix*, whose elements are the first derivatives of $c(x)$ evaluated at x_k. The QP constraints therefore comprise the $n_L + n_N$ linear constraints

$$\begin{array}{rcl} A_L x - s_L & = & 0, \\ c'(x_k)x - s_N & = & -c(x_k) + c'(x_k)x_k, \end{array} \tag{4}$$

where x and s are bounded above and below by u and l as before. If the $(n_L + n_N) \times n$ matrix A and $(n_L + n_N)$-vector b are defined as

$$A = \begin{pmatrix} A_L \\ c'(x_k) \end{pmatrix} \quad \text{and} \quad b = \begin{pmatrix} 0 \\ -c(x_k) + c'(x_k)x_k \end{pmatrix}, \tag{5}$$

then the QP subproblem can be written as

$$\underset{x,s}{\text{minimize}} q(x, x_k) = g_k^{\mathrm{T}}(x - x_k) + \frac{1}{2}(x - x_k)H_k(x - x_k) \quad \text{subject to } Ax - s = b, \quad l \leq \begin{pmatrix} x \\ s \end{pmatrix} \leq u, \tag{6}$$

where $q(x, x_k)$ is a quadratic approximation to a modified Lagrangian function (see Gill *et al.* (2002)). The matrix H_k is a quasi-Newton approximation to the Hessian of the Lagrangian. A BGFS update is applied after each major iteration. If some of the variables enter the Lagrangian linearly the Hessian will have some zero rows and columns. If the nonlinear variables appear first, then only the leading n_N rows and columns of the Hessian need to be approximated.

11.3 Minor Iterations

Solving the QP subproblem is itself an iterative procedure. Here, the iterations of the QP solver nag_opt_sparse_convex_qp_solve (e04nqc) form the *minor* iterations of the SQP method. nag_opt_sparse_convex_qp_solve (e04nqc) uses a reduced-Hessian active-set method implemented as a reduced-gradient method. At each minor iteration, the constraints $Ax - s = b$ are partitioned into the form

$$Bx_B + Sx_S + Nx_N = b, \tag{7}$$

where the *basis matrix* B is square and nonsingular, and the matrices S and N are the remaining columns of $\begin{pmatrix} A & -I \end{pmatrix}$. The vectors x_B, x_S and x_N are the associated *basic*, *superbasic* and *nonbasic* variables respectively; they are a permutation of the elements of x and s. At a QP subproblem, the basic and superbasic variables will lie somewhere between their bounds, while the nonbasic variables will normally be equal to one of their bounds. At each iteration, x_S is regarded as a set of independent variables that are free to move in any desired direction, namely one that will improve the value of the QP objective (or the sum of infeasibilities). The basic variables are then adjusted in order to ensure that (x, s) continues to satisfy $Ax - s = b$. The number of superbasic variables (n_S, say) therefore indicates the number of degrees of freedom remaining after the constraints have been satisfied. In broad terms, n_S is a measure of *how nonlinear* the problem is. In particular, n_S will always be zero for LP problems.

If it appears that no improvement can be made with the current definition of B, S and N, a nonbasic variable is selected to be added to S, and the process is repeated with the value of n_S increased by one. At all stages, if a basic or superbasic variable encounters one of its bounds, the variable is made nonbasic and the value of n_S is decreased by one.

Associated with each of the $n_L + n_N$ equality constraints $Ax - s = b$ are the *dual variables* π. Similarly, each variable in (x, s) has an associated *reduced gradient* d_j. The reduced gradients for the variables x are the quantities $g - A^{\mathrm{T}}\pi$, where g is the gradient of the QP objective, and the reduced gradients for the slacks are the dual variables π. The QP subproblem is optimal if $d_j \geq 0$ for all nonbasic variables at their lower bounds, $d_j \leq 0$ for all nonbasic variables at their upper bounds, and $d_j = 0$ for other variables, including superbasics. In practice, an *approximate* QP solution $(\hat{x}_k, \hat{s}_k, \hat{\pi}_k)$ is found by relaxing these conditions.

11.4 The Merit Function

After a QP subproblem has been solved, new estimates of the solution are computed using a linesearch on the augmented Lagrangian merit function

$$\mathcal{M}(x,s,\pi) = F(x) - \pi^{\mathrm{T}}(c(x) - s_N) + \frac{1}{2}(c(x) - s_N)^{\mathrm{T}} D (c(x) - s_N), \tag{8}$$

where D is a diagonal matrix of penalty arguments ($D_{ii} \geq 0$), and π now refers to dual variables for the nonlinear constraints in (1). If (x_k, s_k, π_k) denotes the current solution estimate and $(\hat{x}_k, \hat{s}_k, \hat{\pi}_k)$ denotes the QP solution, the linesearch determines a step α_k ($0 < \alpha_k \leq 1$) such that the new point

$$\begin{pmatrix} x_{k+1} \\ s_{k+1} \\ \pi_{k+1} \end{pmatrix} = \begin{pmatrix} x_k \\ s_k \\ \pi_k \end{pmatrix} + \alpha_k \begin{pmatrix} \hat{x}_k - x_k \\ \hat{s}_k - s_k \\ \hat{\pi}_k - \pi_k \end{pmatrix} \tag{9}$$

gives a *sufficient decrease* in the merit function $\mathcal{M}$. When necessary, the penalties in D are increased by the minimum-norm perturbation that ensures descent for $\mathcal{M}$ (see Gill *et al.* (1992)). The value of s_N is adjusted to minimize the merit function as a function of s before the solution of the QP subproblem (see Gill *et al.* (1986) and Eldersveld (1991)).

11.5 Treatment of Constraint Infeasibilities

nag_opt_nlp_solve (e04wdc) makes explicit allowance for infeasible constraints. First, infeasible *linear* constraints are detected by solving the linear program

$$\underset{x,v,w}{\text{minimize}} e^{\mathrm{T}}(v+w) \quad \text{subject to } l \leq \begin{pmatrix} x \\ A_L x - v + w \end{pmatrix} \leq u, \quad v \geq 0, \quad w \geq 0, \tag{10}$$

where e is a vector of ones, and the nonlinear constraint bounds are temporarily excluded from l and u. This is equivalent to minimizing the sum of the general linear constraint violations subject to the bounds on x. (The sum is the ℓ_1-norm of the linear constraint violations. In the linear programming literature, the approach is called *elastic programming*.)

The linear constraints are infeasible if the optimal solution of (10) has $v \neq 0$ or $w \neq 0$. nag_opt_nlp_solve (e04wdc) then terminates without computing the nonlinear functions.

Otherwise, all subsequent iterates satisfy the linear constraints. (Such a strategy allows linear constraints to be used to define a region in which the functions can be safely evaluated.) nag_opt_nlp_solve (e04wdc) proceeds to solve nonlinear problems as given, using search directions obtained from the sequence of QP subproblems (see (6)).

If a QP subproblem proves to be infeasible or unbounded (or if the dual variables π for the nonlinear constraints become large), nag_opt_nlp_solve (e04wdc) enters 'elastic' mode and thereafter solves the problem

$$\underset{x,v,w}{\text{minimize}} F(x) + \gamma e^{\mathrm{T}}(v+w) \quad \text{subject to } l \leq \begin{pmatrix} x \\ A_L x \\ c(x) - v + w \end{pmatrix} \leq u, \quad v \geq 0, \quad w \geq 0, \tag{11}$$

where γ is a non-negative argument (the *elastic weight*), and $F(x) + \gamma e^{\mathrm{T}}(v+w)$ is called a *composite objective* (the ℓ_1 penalty function for the nonlinear constraints).

The value of γ may increase automatically by multiples of 10 if the optimal v and w continue to be nonzero. If γ is sufficiently large, this is equivalent to minimizing the sum of the nonlinear constraint violations subject to the linear constraints and bounds.

The initial value of γ is controlled by the optional argument **Elastic Weight**.

12 Optional Arguments

Several optional arguments in nag_opt_nlp_solve (e04wdc) define choices in the problem specification or the algorithm logic. In order to reduce the number of formal arguments of nag_opt_nlp_solve (e04wdc) these optional arguments have associated *default values* that are appropriate for most problems.

Therefore, you need only specify those optional arguments whose values are to be different from their default values.

The remainder of this section can be skipped if you wish to use the default values for all optional arguments.

The following is a list of the optional arguments available. A full description of each optional argument is provided in Section 12.1.

Backup Basis File
Central Difference Interval
Check Frequency
Cold Start
Crash Option
Crash Tolerance
Defaults
Derivative Level
Derivative Linesearch
Difference Interval
Dump File
Elastic Weight
Expand Frequency
Factorization Frequency
Feasibility Tolerance
Feasible Point
Function Precision
Hessian Frequency
Hessian Full Memory
Hessian Limited Memory
Hessian Updates
Infinite Bound Size
Insert File
Iterations Limit
Linesearch Tolerance
List
Load File
LU Complete Pivoting
LU Density Tolerance
LU Factor Tolerance
LU Partial Pivoting
LU Rook Pivoting
LU Singularity Tolerance
LU Update Tolerance
Major Feasibility Tolerance
Major Iterations Limit
Major Optimality Tolerance
Major Print Level
Major Step Limit
Maximize
Minimize

Minor Feasibility Tolerance
Minor Iterations Limit
Minor Print Level
New Basis File
New Superbasics Limit
Nolist
Nonderivative Linesearch
Old Basis File
Partial Price
Pivot Tolerance
Print File
Print Frequency
Proximal Point Method
Punch File
QPSolver CG
QPSolver Cholesky
QPSolver QN
Reduced Hessian Dimension
Save Frequency
Scale Option
Scale Print
Scale Tolerance
Solution File
Start Constraint Check At Variable
Start Objective Check At Variable
Stop Constraint Check At Variable
Stop Objective Check At Variable
Summary File
Summary Frequency
Superbasics Limit
Suppress Parameters
System Information No
System Information Yes
Timing Level
Unbounded Objective
Unbounded Step Size
Verify Level
Violation Limit
Warm Start

Optional arguments may be specified by calling one, or more, of the functions nag_opt_nlp_option_set_file (e04wec), nag_opt_nlp_option_set_string (e04wfc) and nag_opt_nlp_option_set_integer (e04wgc) before a call to nag_opt_nlp_solve (e04wdc).

nag_opt_nlp_option_set_file (e04wec) reads options from an external options file, with `Begin` and `End` as the first and last lines respectively and each intermediate line defining a single optional argument. For example,

```
Begin
   Print Level = 5
End
```

The call

```
nag_opt_nlp_option_set_file(ioptns, &state, &fail);
```

can then be used to read the file on the descriptor `ioptns` as returned by a call of nag_open_file (x04acc). **fail.code** = NE_NOERROR on successful exit. nag_opt_nlp_option_set_file (e04wec) should be consulted for a full description of this method of supplying optional arguments.

nag_opt_nlp_option_set_string (e04wfc), nag_opt_nlp_option_set_integer (e04wgc) or nag_opt_nlp_option_set_double (e04whc) can be called to supply options directly, one call being necessary for each optional argument. nag_opt_nlp_option_set_string (e04wfc), nag_opt_nlp_option_set_integer (e04wgc) or nag_opt_nlp_option_set_double (e04whc) should be consulted for a full description of this method of supplying optional arguments.

All optional arguments not specified by you are set to their default values. Optional arguments specified by you are unaltered by nag_opt_nlp_solve (e04wdc) (unless they define invalid values) and so remain in effect for subsequent calls to nag_opt_nlp_solve (e04wdc), unless altered by you.

12.1 Description of the Optional Arguments

For each option, we give a summary line, a description of the optional argument and details of constraints.

The summary line contains:

the keywords, where the minimum abbreviation of each keyword is underlined (if no characters of an optional qualifier are underlined, the qualifier may be omitted);

a parameter value, where the letters a, i and r denote options that take character, integer and real values respectively;

the default value, where the symbol ϵ is a generic notation for ***machine precision*** (see nag_machine_precision (X02AJC)), and ϵ_r denotes the relative precision of the objective function **Function Precision**, and $bigbnd$ signifies the value of **Infinite Bound Size**.

Keywords and character values are case and white space insensitive.

Optional arguments used to specify files (e.g., optional arguments **Dump File** and **Print File**) have type Nag_FileID (see Section 3.2.1.1 in the Essential Introduction). This ID value must either be set to 0 (the default value) in which case there will be no output, or will be as returned by a call of nag_open_file (x04acc).

Central Difference Interval r Default $= \epsilon_r^{\frac{1}{3}}$

When **Derivative Level** < 3, the central-difference interval r is used near an optimal solution to obtain more accurate (but more expensive) estimates of gradients. Twice as many function evaluations are required compared to forward differencing. The interval used for the jth variable is $h_j = r\left(1 + \left|x_j\right|\right)$. The resulting derivative estimates should be accurate to $O(r^2)$, unless the functions are badly scaled.

If you supply a value for this optional parameter, a small value between 0.0 and 1.0 is appropriate.

Check Frequency i Default $= 60$

Every ith minor iteration after the most recent basis factorization, a numerical test is made to see if the current solution x satisfies the general linear constraints (the linear constraints and the linearized nonlinear constraints, if any). The constraints are of the form $Ax - s = b$, where s is the set of slack variables. To perform the numerical test, the residual vector $r = b - Ax + s$ is computed. If the largest component of r is judged to be too large, the current basis is refactorized and the basic variables are recomputed to satisfy the general constraints more accurately. If $i \leq 0$, the value of $i = 99999999$ is used and effectively no checks are made.

Check Frequency $= 1$ is useful for debugging purposes, but otherwise this option should not be needed.

Cold Start Default
Warm Start

This option controls the specification of the initial working set in the procedure for finding a feasible point for the linear constraints and bounds and in the first QP subproblem thereafter. With a **Cold Start**, the first working set is chosen by nag_opt_nlp_solve (e04wdc) based on the values of the variables and constraints at the initial point. Broadly speaking, the initial working set will include equality constraints and bounds or inequality constraints that violate or 'nearly' satisfy their bounds (to within **Crash Tolerance**).

With a **Warm Start**, you must set the **istate** array and define **clamda** and **h** as discussed in Section 5. **istate** values associated with bounds and linear constraints determine the initial working set of the procedure to find a feasible point with respect to the bounds and linear constraints. **istate** values associated with nonlinear constraints determine the initial working set of the first QP subproblem after such a feasible point has been found. nag_opt_nlp_solve (e04wdc) will override your specification of **istate** if necessary, so that a poor choice of the working set will not cause a fatal error. For instance, any elements of **istate** which are set to -2, -1 or 4 will be reset to zero, as will any elements which are set to 3 when the corresponding elements of **bl** and **bu** are not equal. A warm start will be advantageous if a good estimate of the initial working set is available – for example, when nag_opt_nlp_solve (e04wdc) is called repeatedly to solve related problems.

Crash Option i Default $= 3$
Crash Tolerance r Default $= 0.1$

If a **Cold Start** is specified, an internal Crash procedure is used to select an initial basis from certain rows and columns of the constraint matrix $\begin{pmatrix} A & -I \end{pmatrix}$. The optional argument **Crash Option** i determines which rows and columns of A are eligible initially, and how many times the Crash procedure is called. Columns of $-I$ are used to pad the basis where necessary.

i	**Meaning**
0	The initial basis contains only slack variables: $B = I$.
1	The Crash procedure is called once, looking for a triangular basis in all rows and columns of A.
2	The Crash procedure is called twice (if there are nonlinear constraints). The first call looks for a triangular basis in linear rows, and the iteration proceeds with simplex iterations until the linear constraints are satisfied. The Jacobian is then evaluated for the first major iteration and the Crash procedure is called again to find a triangular basis in the nonlinear rows (retaining the current basis for linear rows).
3	The Crash procedure is called up to three times (if there are nonlinear constraints). The first two calls treat *linear equalities* and *linear inequalities* separately. As before, the last call treats nonlinear rows before the first major iteration.

If $i \geq 1$, certain slacks on inequality rows are selected for the basis first. (If $i \geq 2$, numerical values are used to exclude slacks that are close to a bound). The Crash procedure then makes several passes through the columns of A, searching for a basis matrix that is essentially triangular. A column is assigned to 'pivot' on a particular row if the column contains a suitably large element in a row that has not yet been assigned. (The pivot elements ultimately form the diagonals of the triangular basis.) For remaining unassigned rows, slack variables are inserted to complete the basis.

The **Crash Tolerance** r allows the starting Crash procedure to ignore certain 'small' nonzeros in each column of A. If $a_{\max}$ is the largest element in column j, other nonzeros of a_{ij} in the columns are ignored if $\left|a_{ij}\right| \leq a_{\max} \times r$. (To be meaningful, r must be in the range $0 \leq r < 1$.)

When $r > 0.0$, the basis obtained by the Crash procedure may not be strictly triangular, but it is likely to be nonsingular and almost triangular. The intention is to obtain a starting basis containing more columns of A and fewer (arbitrary) slacks. A feasible solution may be reached sooner on some problems.

For example, suppose the first m columns of A form the matrix shown under **LU Factor Tolerance**; i.e., a tridiagonal matrix with entries -1, 4, -1. To help the Crash procedure choose all m columns for the initial basis, we would specify a **Crash Tolerance** of r for some value of $r > 0.5$.

Defaults

This special keyword may be used to reset all optional arguments to their default values.

Derivative Level i Default $= 3$

Optional argument **Derivative Level** specifies which nonlinear function gradients are known analytically and will be supplied to nag_opt_nlp_solve (e04wdc) by user-supplied functions **objfun** and **confun**.

i	**Meaning**
3	All objective and constraint gradients are known.
2	All constraint gradients are known, but some or all components of the objective gradient are unknown.
1	The objective gradient is known, but some or all of the constraint gradients are unknown.
0	Some components of the objective gradient are unknown and some of the constraint gradients are unknown.

The value $i = 3$ should be used whenever possible. It is the most reliable and will usually be the most efficient.

If $i = 0$ or 2, nag_opt_nlp_solve (e04wdc) will *estimate* the missing components of the objective gradient, using finite differences. This may simplify the coding of **objfun**. However, it could increase the total run-time substantially (since a special call to **objfun** is required for each missing element), and there is less assurance that an acceptable solution will be located. If the nonlinear variables are not well scaled, it may be necessary to specify a non-default optional argument **Difference Interval**.

If $i = 0$ or 1, nag_opt_nlp_solve (e04wdc) will estimate missing elements of the Jacobian. For each column of the Jacobian, one call to **confun** is needed to estimate all missing elements in that column, if any.

At times, central differences are used rather than forward differences. (This is not under your control.)

Derivative Linesearch Default
Nonderivative Linesearch

At each major iteration a linesearch is used to improve the merit function. Optional argument **Derivative Linesearch** uses safeguarded cubic interpolation and requires both function and gradient values to compute estimates of the step α_k. If some analytic derivatives are not provided, or optional argument **Nonderivative Linesearch** is specified, nag_opt_nlp_solve (e04wdc) employs a linesearch based upon safeguarded quadratic interpolation, which does not require gradient evaluations.

A nonderivative linesearch can be slightly less robust on difficult problems, and it is recommended that the default be used if the functions and derivatives can be computed at approximately the same cost. If the gradients are very expensive relative to the functions, a nonderivative linesearch may give a significant decrease in computation time.

If **Nonderivative Linesearch** is selected, nag_opt_nlp_solve (e04wdc) signals the evaluation of the linesearch by calling **objfun** with **mode** $= 0$. If the potential saving provided by a nonderivative linesearch is to be realised, it is essential that **objfun** be coded so that derivatives are not computed when **mode** $= 0$.

Difference Interval r Default $= \sqrt{\epsilon_r}$

This alters the interval r used to estimate gradients by forward differences. It does so in the following circumstances:

– in the interval ('cheap') phase of verifying the problem derivatives;

– for verifying the problem derivatives;

– for estimating missing derivatives.

In all cases, a derivative with respect to x_j is estimated by perturbing that component of x to the value $x_j + r(1 + |x_j|)$, and then evaluating $F(x)$ or $c(x)$ at the perturbed point. The resulting gradient estimates should be accurate to $O(r)$ unless the functions are badly scaled. Judicious alteration of r may sometimes lead to greater accuracy.

If you supply a value for this optional parameter, a small value between 0.0 and 1.0 is appropriate.

Dump File i_1 Default $= 0$
Load File i_2 Default $= 0$

(See Section 3.2.1.1 in the Essential Introduction for further information on NAG data types.)

Optional arguments **Dump File** and **Load File** are similar to optional arguments **Punch File** and **Insert File**, but they record solution information in a manner that is more direct and more easily modified. A full description of information recorded in optional arguments **Dump File** and **Load File** is given in Gill *et al.* (2005a).

If **Dump File** > 0, the last solution obtained will be output to the file associated with ID i_1.

If **Load File** > 0, the file associated with ID i_2, containing basis information, will be read. The file will usually have been output previously as a **Dump File**. The file will not be accessed if optional arguments **Old Basis File** or **Insert File** are specified.

Elastic Weight r Default $= 10^4$

This keyword determines the initial weight γ associated with the problem (11) (see Section 11.5).

At major iteration k, if elastic mode has not yet started, a scale factor $\sigma_k = 1 + \|g(x_k)\|_\infty$ is defined from the current objective gradient. Elastic mode is then started if the QP subproblem is infeasible, or the QP dual variables are larger in magnitude than $\sigma_k r$. The QP is resolved in elastic mode with $\gamma = \sigma_k r$.

Thereafter, major iterations continue in elastic mode until they converge to a point that is optimal for (11) (see Section 11.5). If the point is feasible for equation (1) $(v = w = 0)$, it is declared locally optimal. Otherwise, γ is increased by a factor of 10 and major iterations continue. If γ has already reached a maximum allowable value, equation (1) is declared locally infeasible.

Expand Frequency i Default $= 10000$

This option is part of the anti-cycling procedure designed to make progress even on highly degenerate problems.

For linear models, the strategy is to force a positive step at every iteration, at the expense of violating the bounds on the variables by a small amount. Suppose that the optional argument **Minor Feasibility Tolerance** is δ. Over a period of i iterations, the tolerance actually used by nag_opt_nlp_solve (e04wdc) increases from 0.5δ to δ (in steps of $0.5\delta/i$).

For nonlinear models, the same procedure is used for iterations in which there is only one superbasic variable. (Cycling can occur only when the current solution is at a vertex of the feasible region.) Thus, zero steps are allowed if there is more than one superbasic variable, but otherwise positive steps are enforced.

Increasing i helps reduce the number of slightly infeasible nonbasic variables (most of which are eliminated during a resetting procedure). However, it also diminishes the freedom to choose a large pivot element (see optional argument **Pivot Tolerance**).

Factorization Frequency i Default $= 50$

At most i basis changes will occur between factorizations of the basis matrix.

With linear programs, the basis factors are usually updated every iteration. The default i is reasonable for typical problems. Higher values up to $i = 100$ (say) may be more efficient on well-scaled problems.

When the objective function is nonlinear, fewer basis updates will occur as an optimum is approached. The number of iterations between basis factorizations will therefore increase. During these iterations a test is made regularly (according to the optional argument **Check Frequency**) to ensure that the general

constraints are satisfied. If necessary the basis will be refactorized before the limit of i updates is reached.

Function Precision r Default $= \epsilon^{0.8}$

The *relative function precision* ϵ_r is intended to be a measure of the relative accuracy with which the functions can be computed. For example, if $F(x)$ is computed as 1000.56789 for some relevant x and if the first 6 significant digits are known to be correct, the appropriate value for ϵ_r would be 1.0e−6.

(Ideally the functions $F(x)$ or $c_i(x)$ should have magnitude of order 1. If all functions are substantially *less* than 1 in magnitude, ϵ_r should be the *absolute* precision. For example, if $F(x) = 1.23456789\text{e}{-4}$ at some point and if the first 6 significant digits are known to be correct, the appropriate value for ϵ_r would be 1.0e−10.)

The default value of ϵ_r is appropriate for simple analytic functions.

In some cases the function values will be the result of extensive computation, possibly involving a costly iterative procedure that can provide few digits of precision. Specifying an appropriate **Function Precision** may lead to savings, by allowing the linesearch procedure to terminate when the difference between function values along the search direction becomes as small as the absolute error in the values.

Hessian Full Memory Default if $n \leq 75$
Hessian Limited Memory Default if $n > 75$

These options select the method for storing and updating the approximate Hessian. (nag_opt_nlp_solve (e04wdc) uses a quasi-Newton approximation to the Hessian of the Lagrangian. A BFGS update is applied after each major iteration.)

If **Hessian Full Memory** is specified, the approximate Hessian is treated as a dense matrix and the BFGS updates are applied explicitly. This option is most efficient when the number of variables n is not too large (say, less than 75). In this case, the storage requirement is fixed and one can expect 1-step Q-superlinear convergence to the solution.

Hessian Limited Memory should be used on problems where n is very large. In this case a limited-memory procedure is used to update a diagonal Hessian approximation H_r a limited number of times. (Updates are accumulated as a list of vector pairs. They are discarded at regular intervals after H_r has been reset to their diagonal.)

Hessian Frequency i Default $= 99999999$

If optional argument **Hessian Full Memory** is in effect and i BFGS updates have already been carried out, the Hessian approximation is reset to the identity matrix. (For certain problems, occasional resets may improve convergence, but in general they should not be necessary.)

Hessian Full Memory and **Hessian Frequency** $= 10$ have a similar effect to **Hessian Limited Memory** and **Hessian Updates** $= 10$ (except that the latter retains the current diagonal during resets).

Hessian Updates i Default $=$ **Hessian Frequency** if **Hessian Full Memory**, 10 otherwise

If optional argument **Hessian Limited Memory** is in effect and i BFGS updates have already been carried out, all but the diagonal elements of the accumulated updates are discarded and the updating process starts again.

Broadly speaking, the more updates stored, the better the quality of the approximate Hessian. However, the more vectors stored, the greater the cost of each QP iteration. The default value is likely to give a robust algorithm without significant expense, but faster convergence can sometimes be obtained with significantly fewer updates (e.g., $i = 5$).

Infinite Bound Size r Default $= 10^{20}$

If $r > 0$, r defines the 'infinite' bound $bigbnd$ in the definition of the problem constraints. Any upper bound greater than or equal to $bigbnd$ will be regarded as $+\infty$ (and similarly any lower bound less than or equal to $-bigbnd$ will be regarded as $-\infty$). If $r < 0$, the default value is used.

Iterations Limit i Default $= \max(10000, 10\max(n, n_L + n_N))$

The value of i specifies the maximum number of minor iterations allowed (i.e., iterations of the simplex method or the QP algorithm), summed over all major iterations. (See also the description of the optional argument **Minor Iterations Limit**.)

Linesearch Tolerance r Default $= 0.9$

This tolerance, r, controls the accuracy with which a step length will be located along the direction of search each iteration. At the start of each linesearch a target directional derivative for the merit function is identified. This argument determines the accuracy to which this target value is approximated, and it must be a value in the range $0.0 \leq r \leq 1.0$.

The default value $r = 0.9$ requests just moderate accuracy in the linesearch.

If the nonlinear functions are cheap to evaluate, a more accurate search may be appropriate; try $r = 0.1$, 0.01 or 0.001.

If the nonlinear functions are expensive to evaluate, a less accurate search may be appropriate. *If all gradients are known*, try $r = 0.99$. (The number of major iterations might increase, but the total number of function evaluations may decrease enough to compensate.)

If not all gradients are known, a moderately accurate search remains appropriate. Each search will require only 1–5 function values (typically), but many function calls will then be needed to estimate missing gradients for the next iteration.

Nolist Default
List

For nag_opt_nlp_solve (e04wdc), normally each optional argument specification is printed as it is supplied. Optional argument **Nolist** may be used to suppress the printing and optional argument **List** may be used to turn on printing.

LU Density Tolerance r_1 Default $= 0.6$
LU Singularity Tolerance r_2 Default $= \epsilon^{\frac{2}{3}}$

The density tolerance, r_1, is used during LU factorization of the basis matrix B. Columns of L and rows of U are formed one at a time, and the remaining rows and columns of the basis are altered appropriately. At any stage, if the density of the remaining matrix exceeds r_1, the Markowitz strategy for choosing pivots is terminated, and the remaining matrix is factored by a dense LU procedure. Raising the density tolerance towards 1.0 may give slightly sparser LU factors, with a slight increase in factorization time.

The singularity tolerance, r_2, helps guard against ill-conditioned basis matrices. After B is refactorized, the diagonal elements of U are tested as follows: if $\left|u_{jj}\right| \leq r_2$ or $\left|u_{jj}\right| < r_2 \max_i \left|u_{ij}\right|$, the jth column of the basis is replaced by the corresponding slack variable. (This is most likely to occur after a restart.)

LU Factor Tolerance r_1 Default $= 1.10$
LU Update Tolerance r_2 Default $= 1.10$

The values of r_1 and r_2 affect the stability of the basis factorization $B = LU$, during refactorization and updates respectively. The lower triangular matrix L is a product of matrices of the form

$$\begin{pmatrix} 1 & \\ \mu & 1 \end{pmatrix}$$

where the multipliers μ will satisfy $|\mu| \leq r_i$. The default values of r_1 and r_2 usually strike a good compromise between stability and sparsity. They must satisfy r_1, $r_2 \geq 1.0$.

For large and relatively dense problems, $r_1 = 10.0$ or 5.0 (say) may give a useful improvement in stability without impairing sparsity to a serious degree.

For certain very regular structures (e.g., band matrices) it may be necessary to reduce r_1 and/or r_2 in order to achieve stability. For example, if the columns of A include a sub-matrix of the form

$$\begin{pmatrix} 4 & -1 & & & & \\ -1 & 4 & -1 & & & \\ & -1 & 4 & -1 & & \\ & & \cdots & \cdots & \cdots & \\ & & & -1 & 4 & -1 \\ & & & & -1 & 4 \end{pmatrix},$$

one should set both r_1 and r_2 to values in the range $1.0 \leq r_i < 4.0$.

LU Partial Pivoting Default
LU Complete Pivoting
LU Rook Pivoting

The LU factorization implements a Markowitz-type search for pivots that locally minimize the fill-in subject to a threshold pivoting stability criterion. The default option is to use threshhold partial pivoting. The optional arguments **LU Rook Pivoting** and **LU Complete Pivoting** are more expensive than partial pivoting but are more stable and better at revealing rank, as long as **LU Factor Tolerance** is not too large (say < 2.0). When numerical difficulties are encountered, nag_opt_nlp_solve (e04wdc) automatically reduces the LU tolerance towards 1.0 and switches (if necessary) to rook or complete pivoting, before reverting to the default or specified options at the next refactorization (with **System Information Yes**, relevant messages are output to the **Print File**).

Major Feasibility Tolerance r Default $= \max\left(10^{-6}, \sqrt{\epsilon}\right)$

This tolerance, r, specifies how accurately the nonlinear constraints should be satisfied. The default value is appropriate when the linear and nonlinear constraints contain data to about that accuracy.

Let $v_{\max}$ be the maximum nonlinear constraint violation, normalized by the size of the solution, which is required to satisfy

$$v_{\max/} = \max_i v_i / \|x\| \leq r, \tag{12}$$

where v_i is the violation of the ith nonlinear constraint $(i = 1 : n_L)$.

In the major iteration log (see Section 13.2, $v_{\max}$ appears as the quantity labelled 'Feasible'. If some of the problem functions are known to be of low accuracy, a larger **Major Feasibility Tolerance** may be appropriate.

Major Optimality Tolerance r Default $= 2\max\left(10^{-6}, \sqrt{\epsilon}\right)$

This tolerance, r, specifies the final accuracy of the dual variables. On successful termination, nag_opt_nlp_solve (e04wdc) will have computed a solution (x, s, π) such that

$$c_{\max} = \max_j c_j / \|\pi\| \leq r, \tag{13}$$

where c_j is an estimate of the complementarity slackness for variable j where $j = 1 : n + n_L + n_N$. The values c_i are computed from the final QP solution using the reduced gradients $d_j = g_j - \pi^{\mathrm{T}} a_j$ (where g_j is the jth component of the objective gradient, a_j is the associated column of the constraint matrix $\begin{pmatrix} A & -I \end{pmatrix}$, and π is the set of QP dual variables):

$$c_j = \begin{cases} d_j \min\left(x_j - l_j, 1\right) & \text{if } d_j \geq 0; \\ -d_j \min\left(u_j - x_j, 1\right) & \text{if } d_j < 0. \end{cases} \tag{14}$$

In the **Print File**, $c_{\max}$ appears as the quantity labelled 'Optimal'.

Major Iterations Limit i Default $= \max(1000, 3\max(n, n_L + n_N))$

This is the maximum number of major iterations allowed. It is intended to guard against an excessive number of linearizations of the constraints. If $i = 0$, optimality and feasibility are checked.

Major Print Level i Default $= 000001$

This controls the amount of output to the optional arguments **Print File** and **Summary File** at each major iteration. **Major Print Level** $= 0$ suppresses most output, except for error messages. **Major Print Level** $= 1$ gives normal output for linear and nonlinear problems, and **Major Print Level** $= 11$ gives additional details of the Jacobian factorization that commences each major iteration.

In general, the value being specified may be thought of as a binary number of the form

Major Print Level $JFDXbs$

where each letter stands for a digit that is either 0 or 1 as follows:

s a single line that gives a summary of each major iteration. (This entry in $JFDXbs$ is not strictly binary since the summary line is printed whenever $JFDXbs \geq 1$);

b basis statistics, i.e., information relating to the basis matrix whenever it is refactorized. (This output is always provided if $JFDXbs \geq 10$);

X x_k, the nonlinear variables involved in the objective function or the constraints. These appear under the heading 'Jacobian variables';

D π_k, the dual variables for the nonlinear constraints. These appear under the heading 'Multiplier estimates';

F $c(x_k)$, the values of the nonlinear constraint functions;

J $J(x_k)$, the Jacobian matrix. This appears under the heading 'x and Jacobian'.

To obtain output of any items $JFDXbs$, set the corresponding digit to 1, otherwise to 0.

If $J = 1$, the Jacobian matrix will be output column-wise at the start of each major iteration. Column j will be preceded by the value of the corresponding variable x_j and a key to indicate whether the variable is basic, superbasic or nonbasic. (Hence if $J = 1$, there is no reason to specify $X = 1$ unless the objective contains more nonlinear variables than the Jacobian.) A typical line of output is

```
3 1.250000e+01 BS 1 1.00000e+00 4 2.00000e+00
```

which would mean that x_3 is basic at value 12.5, and the third column of the Jacobian has elements of 1.0 and 2.0 in rows 1 and 4.

Major Step Limit r Default $= 2.0$

This argument limits the change in x during a linesearch. It applies to all nonlinear problems, once a 'feasible solution' or 'feasible subproblem' has been found. A linesearch determines a step α over the range $0 < \alpha \leq \beta$, where β is 1 if there are nonlinear constraints, or is the step to the nearest upper or lower bound on x if all the constraints are linear. Normally, the first step length tried is $\alpha_1 = \min(1, \beta)$.

1. In some cases, such as $f(x) = ae^{bx}$ or $f(x) = ax^b$, even a moderate change in the components of x can lead to floating-point overflow. The argument r is therefore used to define a limit $\bar{\beta} = r(1 + \|x\|)/\|p\|$ (where p is the search direction), and the first evaluation of $f(x)$ is at the potentially smaller step length $\alpha_1 = \min(1, \bar{\beta}, \beta)$.
2. Wherever possible, upper and lower bounds on x should be used to prevent evaluation of nonlinear functions at meaningless points. The optional argument **Major Step Limit** provides an additional safeguard. The default value $r = 2.0$ should not affect progress on well behaved problems, but setting $r = 0.1$ or 0.01 may be helpful when rapidly varying functions are present. A 'good' starting point may be required. An important application is to the class of nonlinear least squares problems.
3. In cases where several local optima exist, specifying a small value for r may help locate an optimum near the starting point.

Minimize Default
Maximize
Feasible Point

The keywords **Minimize** and **Maximize** specify the required direction of optimization. It applies to both linear and nonlinear terms in the objective.

The keyword **Feasible Point** means 'Ignore the objective function, while finding a feasible point for the linear and nonlinear constraints'. It can be used to check that the nonlinear constraints are feasible without altering the call to nag_opt_nlp_solve (e04wdc).

Minor Feasibility Tolerance
Feasibility Tolerance r Default $= \max\{10^{-6}, \sqrt{\epsilon}\}$

nag_opt_nlp_solve (e04wdc) tries to ensure that all variables eventually satisfy their upper and lower bounds to within this tolerance, r. This includes slack variables. Hence, general linear constraints should also be satisfied to within r.

Feasibility with respect to nonlinear constraints is judged by the optional argument **Major Feasibility Tolerance** (not by r).

If the bounds and linear constraints cannot be satisfied to within r, the problem is declared *infeasible*. If the corresponding sum of infeasibilities is quite small, it may be appropriate to raise r by a factor of 10 or 100. Otherwise, some error in the data should be suspected.

Nonlinear functions will be evaluated only at points that satisfy the bounds and linear constraints. If there are regions where a function is undefined, every attempt should be made to eliminate these regions from the problem.

For example, if $f(x) = \sqrt{x_1} + \log(x_2)$, it is essential to place lower bounds on both variables. If $r = 1.0\text{e}{-6}$, the bounds $x_1 \geq 10^{-5}$ and $x_2 \geq 10^{-4}$ might be appropriate. (The log singularity is more serious. In general, keep x as far away from singularities as possible.)

If **Scale Option** ≥ 1, feasibility is defined in terms of the *scaled* problem (since it is then more likely to be meaningful).

In reality, nag_opt_nlp_solve (e04wdc) uses r as a feasibility tolerance for satisfying the bounds on x and s in each QP subproblem. If the sum of infeasibilities cannot be reduced to zero, the QP subproblem is declared infeasible. nag_opt_nlp_solve (e04wdc) is then in *elastic mode* thereafter (with only the linearized nonlinear constraints defined to be elastic). See the description of the optional argument **Elastic Weight**.

Minor Iterations Limit i Default $= 500$

If the number of minor iterations for the optimality phase of the QP subproblem exceeds i, then all nonbasic QP variables that have not yet moved are frozen at their current values and the reduced QP is solved to optimality.

Note that more than i minor iterations may be necessary to solve the reduced QP to optimality. These extra iterations are necessary to ensure that the terminated point gives a suitable direction for the linesearch.

In the major iteration log (see Section 13.2) a `t` at the end of a line indicates that the corresponding QP was artificially terminated using the limit i.

Compare with the optional argument **Iterations Limit**, which defines an independent *absolute* limit on the *total* number of minor iterations (summed over all QP subproblems).

Minor Print Level i Default $= 1$

This controls the amount of output to the **Print File** and the **Summary File** during solution of the QP subproblems. The value of i has the following effect:

i	Output
0	No minor iteration output except error messages.

≥ 1 A single line of output at each minor iteration (controlled by optional arguments **Print Frequency** and **Summary Frequency**.

≥ 10 Basis factorization statistics generated during the periodic refactorization of the basis (see the optional argument **Factorization Frequency**). Statistics for the *first factorization* each major iteration are controlled by the optional argument **Major Print Level**.

New Basis File	i_1	Default $= 0$
Backup Basis File	i_2	Default $= 0$
Save Frequency	i_3	Default $= 100$

(See Section 3.2.1.1 in the Essential Introduction for further information on NAG data types.)

New Basis File and **Backup Basis File** are sometimes referred to as basis maps. They contain the most compact representation of the state of each variable. They are intended for restarting the solution of a problem at a point that was reached by an earlier run. For nontrivial problems, it is advisable to save basis maps at the end of a run, in order to restart the run if necessary.

If **New Basis File** > 0, a basis map will be saved on the **New Basis File** every i_3th iteration. The first record of the file will contain the word `PROCEEDING` if the run is still in progress. A basis map will also be saved at the end of a run, with some other word indicating the final solution status.

If **Backup Basis File** > 0, it is intended as a safeguard against losing the results of a long run. Suppose that a **New Basis File** is being saved every 100 (**Save Frequency**) iterations, and that nag_opt_nlp_solve (e04wdc) is about to save such a basis at iteration 2000. It is conceivable that the run may be interrupted during the next few milliseconds (in the middle of the save). In this case the Basis file will be corrupted and the run will have been essentially wasted.

To eliminate this risk, both a **New Basis File** and a **Backup Basis File** may be specified using calls of nag_open_file (x04acc).

The current basis will then be saved every 100 iterations, first on the **New Basis File** and then immediately on the **Backup Basis File**. If the run is interrupted at iteration 2000 during the save on the **New Basis File**, there will still be a usable basis on the **Backup Basis File** (corresponding to iteration 1900).

Note that a new basis will be saved in **New Basis File** at the end of a run if it terminates normally, but it will not be saved in **Backup Basis File**. In the above example, if an optimum solution is found at iteration 2050 (or if the iteration limit is 2050), the final basis in the **New Basis File** will correspond to iteration 2050, but the last basis saved in the **Backup Basis File** will be the one for iteration 2000.

A full description of information recorded in **New Basis File** and **Backup Basis File** is given in Gill *et al.* (2005a).

New Superbasics Limit i Default $= 99$

This option causes early termination of the QP subproblems if the number of free variables has increased significantly since the first feasible point. If the number of new superbasics is greater than i, the nonbasic variables that have not yet moved are frozen and the resulting smaller QP is solved to optimality.

In the major iteration log (see Section 13.1), a `t` at the end of a line indicates that the QP was terminated early in this way.

Old Basis File i Default $= 0$

(See Section 3.2.1.1 in the Essential Introduction for further information on NAG data types.)

If **Old Basis File** > 0, the basis maps information will be obtained from the file associated with ID i. The file will usually have been output previously as a **New Basis File** or **Backup Basis File**. A full description of information recorded in **New Basis File** and **Backup Basis File** is given in Gill *et al.* (2005a).

The file will not be acceptable if the number of rows or columns in the problem has been altered.

Partial Price i Default $= 1$

This argument is recommended for large problems that have significantly more variables than constraints. It reduces the work required for each 'pricing' operation (where a nonbasic variable is selected to become superbasic). When $i = 1$, all columns of the constraint matrix $\begin{pmatrix} A & -I \end{pmatrix}$ are searched. Otherwise, A and I are partitioned to give i roughly equal segments A_j and I_j, for $j = 1, 2, \ldots, i$. If the previous pricing search was successful on A_{j-1} and I_{j-1}, the next search begins on the segments A_j and I_j. (All subscripts here are modulo i.) If a reduced gradient is found that is larger than some dynamic tolerance, the variable with the largest such reduced gradient (of appropriate sign) is selected to become superbasic. If nothing is found, the search continues on the next segments A_{j+1} and I_{j+1}, and so on.

For time-stage models having t time periods, **Partial Price** t (or $t/2$ or $t/3$) may be appropriate.

Pivot Tolerance r Default $= \epsilon^{\frac{2}{3}}$

During the solution of QP subproblems, the pivot tolerance is used to prevent columns entering the basis if they would cause the basis to become almost singular.

When x changes to $x + \alpha p$ for some search direction p, a 'ratio test' determines which component of x reaches an upper or lower bound first. The corresponding element of p is called the pivot element. Elements of p are ignored (and therefore cannot be pivot elements) if they are smaller than the pivot tolerance r.

It is common for two or more variables to reach a bound at essentially the same time. In such cases, the **Minor Feasibility Tolerance** (say, t) provides some freedom to maximize the pivot element and thereby improve numerical stability. Excessively small values of t should therefore not be specified. To a lesser extent, the **Expand Frequency** (say, f) also provides some freedom to maximize the pivot element. Excessively *large* values of f should therefore not be specified.

Print File i Default $= 0$

(See Section 3.2.1.1 in the Essential Introduction for further information on NAG data types.)

If **Print File** > 0, the following information is output to a file associated with ID i during the solution of each problem:

– a listing of the optional arguments;

– some statistics about the problem;

– the amount of storage available for the LU factorization of the basis matrix;

– notes about the initial basis resulting from a Crash procedure or a Basis file;

– the iteration log;

– basis factorization statistics;

– the exit **fail** condition and some statistics about the solution obtained;

– the printed solution, if requested.

These items are described in Sections 9 and 13. Further brief output may be directed to the **Summary File**.

Print Frequency i Default $= 100$

If $i > 0$, one line of the iteration log will be printed every ith iteration. A value such as $i = 10$ is suggested for those interested only in the final solution. If $i \leq 0$, the value of $i = 99999999$ is used and effectively no checks are made.

Proximal Point Method i Default $= 1$

$i = 1$ or 2 specifies minimization of $\|x - x_0\|_1$ or $\frac{1}{2}\|x - x_0\|_2^2$ when the starting point x_0 is changed to satisfy the linear constraints (where x_0 refers to nonlinear variables).

Punch File i_1 Default $= 0$
Insert File i_2 Default $= 0$

(See Section 3.2.1.1 in the Essential Introduction for further information on NAG data types.)

The **Punch File** from a previous run may be used as an **Insert File** for a later run on the same problem. A full description of information recorded in **Insert File** and **Punch File** is given in Gill *et al.* (2005a).

If **Punch File** > 0, the final solution obtained will be output to the file associated with ID i_1. For linear programs, this format is compatible with various commercial systems.

If **Insert File** > 0, the file associated with ID i_2, containing basis information, will be read. The file will usually have been output previously as a **Punch File**. The file will not be accessed if **Old Basis File** is specified.

QPSolver Cholesky Default
QPSolver CG
QPSolver QN

Specifies the active-set algorithm used to solve subproblem (11) (see Section 11.5). **QPSolver Cholesky** holds the full Cholesky factor R of the reduced Hessian $Z^{\mathrm{T}}HZ$. As the QP iterations proceed, the dimension of R changes with the number of superbasic variables. If the number of superbasic variables needs to increase beyond the value of **Reduced Hessian Dimension**, the reduced Hessian cannot be stored and the solver switches to **QPSolver CG**. The Cholesky solver is reactivated if the number of superbasics stabilizes at a value less than **Reduced Hessian Dimension**.

QPSolver QN solves the QP using a quasi-Newton method. In this case, R is the factor of a quasi-Newton approximate Hessian.

QPSolver CG uses an active-set method similar to **QPSolver QN**, but uses the conjugate-gradient method to solve all systems involving the reduced Hessian.

The Cholesky QP solver is the most robust, but may require a significant amount of computation if there are many superbasics.

The quasi-Newton QP solver does not require computation of the exact R at the start of the subproblem in (11). It may be appropriate when the number of superbasics is large but relatively few iterations are needed to reach a solution (e.g., if nag_opt_nlp_solve (e04wdc) is called with a Warm Start).

The conjugate-gradient QP solver is appropriate for problems with many degrees of freedom (say, more than 2000 superbasics).

Reduced Hessian Dimension i Default $= \min(2000, n)$

This specifies that an i by i triangular matrix R (to define the reduced Hessian according to $R^{\mathrm{T}}R = Z^{\mathrm{T}}HZ$) is to be available for use by the Cholesky QP solver.

Scale Option i Default $= 0$
Scale Tolerance r Default $= 0.9$
Scale Print

Three scale options are available as follows:

i	**Meaning**
0	No scaling. This is recommended if it is known that x and the constraint matrix never have very large elements (say, larger than 100).

1 The constraints and variables are scaled by an iterative procedure that attempts to make the matrix coefficients as close as possible to 1.0 (see Fourer (1982)). This will sometimes improve the performance of the solution procedures.

2 The constraints and variables are scaled by the iterative procedure. Also, a certain additional scaling is performed that may be helpful if the right-hand side b or the solution x is large. This takes into account columns of $\begin{pmatrix} A & -I \end{pmatrix}$ that are fixed or have positive lower bounds or negative upper bounds.

Optional argument **Scale Tolerance** affects how many passes might be needed through the constraint matrix. On each pass, the scaling procedure computes the ratio of the largest and smallest nonzero coefficients in each column:

$$\rho_j = \max_j |a_{ij}| / \min_i |a_{ij}| \quad (a_{ij} \neq 0).$$

If $\max_j \rho_j$ is less than r times its previous value, another scaling pass is performed to adjust the row and column scales. Raising r from 0.9 to 0.99 (say) usually increases the number of scaling passes through A. At most 10 passes are made. The value of r should lie in the range $0 < r < 1$.

Scale Print causes the row scales $r(i)$ and column scales $c(j)$ to be printed to **Print File**, if **System Information Yes** has been specified. The scaled matrix coefficients are $\bar{a}_{ij} = a_{ij}c(j)/r(i)$, and the scaled bounds on the variables and slacks are $\bar{l}_j = l_j/c(j)$, $\bar{u}_j = u_j/c(j)$, where $c(j) = r(j-n)$ if $j > n$.

Solution File i Default $= 0$

(See Section 3.2.1.1 in the Essential Introduction for further information on NAG data types.)

If **Solution File** > 0, the final solution will be output to the file associated with ID i.

To see more significant digits in the printed solution, it will sometimes be useful to specify that the **Solution File** refers to the **Print File**.

Start Objective Check At Variable i Default $= 1$
Stop Objective Check At Variable i Default $= n$
Start Constraint Check At Variable i Default $= 1$
Stop Constraint Check At Variable i Default $= n$

These keywords take effect only if **Verify Level** > 0. They may be used to contol the verification of gradient elements computed by function **objfun** and/or Jacobian elements computed by function **confun**. For eample, if the first 30 elements of the objective gradient appeared to be correct in an earlier run, so that only element 31 remains questionable, it is reasonable to specify **Start Objective Check At Variable** $= 31$. If the first 30 variables appear linearly in the objective, so that the corresponding gradient elements are constant, the above choice would also be appropriate.

Summary File i_1 Default $= 0$
Summary Frequency i_2 Default $= 100$

(See Section 3.2.1.1 in the Essential Introduction for further information on NAG data types.)

If **Summary File** > 0, a brief log will be output to the file associated with i_1, including one line of information every i_2th iteration. In an interactive environment, it is useful to direct this output to the terminal, to allow a run to be monitored online. (If something looks wrong, the run can be manually terminated.) Further details are given in Section 13.6.

Superbasics Limit i Default $= n$

This option places a limit on the storage allocated for superbasic variables. Ideally, i should be set slightly larger than the 'number of degrees of freedom' expected at an optimal solution.

For nonlinear problems, the number of degrees of freedom is often called the 'number of independent variables'. Normally, i need not be greater than $n_N + 1$, where n_N is the number of nonlinear variables. For many problems, i may be considerably smaller than n_N. This will save storage if n_N is very large.

Suppress Parameters

Normally nag_opt_nlp_solve (e04wdc) prints the options file as it is being read, and then prints a complete list of the available keywords and their final values. The optional argument **Suppress Parameters** tells nag_opt_nlp_solve (e04wdc) not to print the full list.

System Information No Default
System Information Yes

This option prints additional information on the progress of major and minor iterations, and Crash statistics. See Section 13.

Timing Level i Default $= 0$

If $i > 0$, some timing information will be output to the Print file, if **Print File** > 0.

Unbounded Objective r_1 Default $= 1.0\text{e}+15$
Unbounded Step Size r_2 Default $= bigbnd$

These arguments are intended to detect unboundedness in nonlinear problems. During a linesearch, F is evaluated at points of the form $x + \alpha p$, where x and p are fixed and α varies. If $|F|$ exceeds r_1 or α exceeds r_2, iterations are terminated with the exit message **fail.code** = NE_UNBOUNDED.

If singularities are present, unboundedness in $F(x)$ may be manifested by a floating-point overflow (during the evaluation of $F(x + \alpha p)$), before the test against r_1 can be made.

Unboundedness in x is best avoided by placing finite upper and lower bounds on the variables.

Verify Level i Default $= 0$

This option refers to finite difference checks on the derivatives computed by the user-supplied functions. Derivatives are checked at the first point that satisfies all bounds and linear constraints.

i	**Meaning**
0	Only a 'cheap' test will be performed, requiring two calls to **confun**.
1	Individual gradients will be checked (with a more reliable test). A key of the form `OK` or `Bad?` indicates whether or not each component appears to be correct.
2	Individual columns of the problem Jacobian will be checked.
3	Options 2 and 1 will both occur (in that order).
-1	Derivative checking is disabled.

Verify Level $= 3$ should be specified whenever a new user function is being developed. Missing derivatives are not checked, so they result in no overhead.

Violation Limit r Default $= 1.0\text{e}+6$

This keyword defines an absolute limit on the magnitude of the maximum constraint violation, r, after the linesearch. On completion of the linesearch, the new iterate x_{k+1} satisfies the condition

$$v_i(x_{k+1}) \leq r \ \max(1, v_i(x_0)),$$

where x_0 is the point at which the nonlinear constraints are first evaluated and $v_i(x)$ is the ith nonlinear constraint violation $v_i(x) = \max(0, l_i - c_i(x), c_i(x) - u_i)$.

The effect of this violation limit is to restrict the iterates to lie in an *expanded* feasible region whose size depends on the magnitude of r. This makes it possible to keep the iterates within a region where the objective is expected to be well defined and bounded below. If the obective is bounded below for all values of the variables, then r may be any large positive value.

13 Description of Monitoring Information

nag_opt_nlp_solve (e04wdc) produces monitoring information, statistical information and information about the solution. Section 9.1 contains the final output information sent to unit **Print File**. This section contains other output information.

13.1 Major Iteration Log

This section describes the output to unit **Print File** if **Major Print Level** > 0. One line of information is output every kth major iteration, where k is **Print Frequency**.

Label	**Description**
`Itns`	is the cumulative number of minor iterations.
`Major`	is the current major iteration number.
`Minors`	is the number of iterations required by both the feasibility and optimality phases of the QP subproblem. Generally, `Minors` will be 1 in the later iterations, since theoretical analysis predicts that the correct active set will be identified near the solution (see Section 11).
`Step`	is the step length α taken along the current search direction p. The variables x have just been changed to $x + \alpha p$. On reasonably well-behaved problems, the unit step will be taken as the solution is approached.
`nCon` or `nObj`	`nCon` is the number of times **confun** has been called to evaluate the nonlinear problem functions. Evaluations needed for the estimation of the derivatives by finite differences are not included. `nCon` is printed as a guide to the amount of work required for the linesearch. If n_N, the number of nonlinear constraints, is zero, `nCon` does not appear, but is replaced by `nObj`. This quantity is the number of calls made to **objfun**.
`Feasible`	is the value of $v_{\max}$ (see (12)), the maximum component of the scaled nonlinear constraint residual (see the description of the optional argument **Major Feasibility Tolerance**). The solution is regarded as acceptably feasible if `Feasible` is less than the **Major Feasibility Tolerance**. In this case, the entry is contained in parentheses. If the constraints are linear, all iterates are feasible and this entry is not printed.
`Optimal`	is the value of $c_{\max}$ (see (13)), the maximum complementary gap (see the description of the optional argument **Major Optimality Tolerance**). It is an estimate of the degree of nonoptimality of the reduced costs. Both `Feasible` and `Optimal` are small in the neighbourhood of a solution.
`MeritFunction` or `Objective`	is the value of the augmented Lagrangian merit function (see (8)). This function will decrease at each iteration unless it was necessary to increase the penalty arguments (see Section 11.4). As the solution is approached, `MeritFunction` will converge to the value of the objective at the solution. In elastic mode, the merit function is a composite function involving the constraint violations weighted by the elastic weight. If the constraints are linear, this item is labelled `Objective`, the value of the objective function. It will decrease monotonically to its optimal value.
`L+U`	is the number of nonzeros representing the basis factors L and U on completion of the QP subproblem. If nonlinear constraints are present, the basis factorization $B = LU$ is computed at the start of the first minor iteration. At this stage, `L+U` $=$ `lenL` $+$ `lenU`, where `lenL` (see Section 13.4) is the number of subdiagonal elements in the columns of a lower triangular matrix and `lenU` (see Section 13.4) is the number of diagonal and superdiagonal elements in the rows of an upper-triangular matrix.

As columns of B are replaced during the minor iterations, `L+U` may fluctuate up or down but, in general, will tend to increase. As the solution is approached and the minor iterations decrease towards zero, `L+U` will reflect the number of nonzeros in the LU factors at the start of the QP subproblem.

If the constraints are linear, refactorization is subject only to the **Factorization Frequency**, and `L+U` will tend to increase between factorizations.

`BSwap` is the number of columns of the basis matrix B that were swapped with columns of S to improve the condition of B. The swaps are determined by an LU factorization of the rectangular matrix $B_S = \begin{pmatrix} B & S \end{pmatrix}^{\mathrm{T}}$ with stability being favoured more than sparsity.

`nS` is the current number of superbasic variables.

`condHz` is an estimate of the condition number of $R^{\mathrm{T}}R$, itself an estimate of $Z^{\mathrm{T}}HZ$, the reduced Hessian of the Lagrangian. The condition number is the square of the ratio of the largest and smallest diagonals of the upper triangular matrix R, this being a lower bound on the condition number of $R^{\mathrm{T}}R$. `condHz` gives a rough indication of whether or not the optimization procedure is having difficulty. If ϵ is the relative ***machine precision*** being used, the SQP algorithm will make slow progress if `condHz` becomes as large as $\epsilon^{-1/2} \approx 10^8$, and will probably fail to find a better solution if `condHz` reaches $\epsilon^{-3/4} \approx 10^{12}$.

To guard against high values of `condHz`, attention should be given to the scaling of the variables and the constraints. In some cases it may be necessary to add upper or lower bounds to certain variables to keep them a reasonable distance from singularities in the nonlinear functions or their derivatives.

`Penalty` is the Euclidean norm of the vector of penalty arguments used in the augmented Lagrangian merit function (not printed if there are no nonlinear constraints).

The summary line may include additional code characters that indicate what happened during the course of the major iteration. These will follow the separator '`_`' in the output.

Label	**Description**
`c`	central differences have been used to compute the unknown components of the objective and constraint gradients. A switch to central differences is made if either the linesearch gives a small step, or x is close to being optimal. In some cases, it may be necessary to re-solve the QP subproblem with the central difference gradient and Jacobian.
`d`	during the linesearch it was necessary to decrease the step in order to obtain a maximum constraint violation conforming to the value of **Violation Limit**.
`D`	you set **mode** $= -1$ on exit from **objfun**, indicating that the linesearch needed to be done with a smaller value of the step length α.
`l`	the norm wise change in the variables was limited by the value of the **Major Step Limit**. If this output occurs repeatedly during later iterations, it may be worthwhile increasing the value of **Major Step Limit**.
`i`	if nag_opt_nlp_solve (e04wdc) is not in elastic mode, an `i` signifies that the QP subproblem is infeasible. This event triggers the start of nonlinear elastic mode, which remains in effect for all subsequent iterations. Once in elastic mode, the QP subproblems are associated with the elastic problem (11) (see Section 11.5). If nag_opt_nlp_solve (e04wdc) is already in elastic mode, an `i` indicates that the minimizer of the elastic subproblem does not satisfy the linearized constraints. (In this case, a feasible point for the usual QP subproblem may or may not exist.)
`M`	an extra evaluation of the problem functions was needed to define an acceptable positive definite quasi-Newton update to the Lagrangian Hessian. This modification is only done when there are nonlinear constraints.

m	this is the same as M except that it was also necessary to modify the update to include an augmented Lagrangian term.
n	no positive definite BFGS update could be found. The approximate Hessian is unchanged from the previous iteration.
R	the approximate Hessian has been reset by discarding all but the diagonal elements. This reset will be forced periodically by the **Hessian Frequency** and **Hessian Updates** keywords. However, it may also be necessary to reset an ill-conditioned Hessian from time to time.
r	the approximate Hessian was reset after ten consecutive major iterations in which no BFGS update could be made. The diagonals of the approximate Hessian are retained if at least one update has been done since the last reset. Otherwise, the approximate Hessian is reset to the identity matrix.
s	a self-scaled BFGS update was performed. This update is used when the Hessian approximation is diagonal, and hence always follows a Hessian reset.
t	the minor iterations were terminated because of the **Minor Iterations Limit**.
T	the minor iterations were terminated because of the **New Superbasics Limit**.
u	the QP subproblem was unbounded.
w	a weak solution of the QP subproblem was found.
z	the **Superbasics Limit** was reached.

13.2 Minor Iteration Log

If **Minor Print Level** > 0, one line of information is output to the Print file every kth minor iteration, where k is the specified **Print Frequency**. A heading is printed before the first such line following a basis factorization. The heading contains the items described below. In this description, a pricing operation is the process by which a nonbasic variable is selected to become superbasic (in addition to those already in the superbasic set). The selected variable is denoted by jq. Variable jq often becomes basic immediately. Otherwise it remains superbasic, unless it reaches its opposite bound and returns to the nonbasic set.

If **Partial Price** is in effect, variable jq is selected from A_{pp} or I_{pp}, the ppth segments of the constraint matrix $\begin{pmatrix} A & -I \end{pmatrix}$.

Label	**Description**
Itn	the current iteration number.
LPmult or QPmult	is the reduced cost (or reduced gradient) of the variable jq selected by the pricing procedure at the start of the present iteration. Algebraically, the reduced gradient is $d_j = g_j - \pi^{\mathrm{T}} a_j$ for $j =$ jq, where g_j is the gradient of the current objective function, π is the vector of dual variables for the QP subproblem, and a_j is the jth column of $\begin{pmatrix} A & -I \end{pmatrix}$. Note that the reduced cost is the 1-norm of the reduced-gradient vector at the start of the iteration, just after the pricing procedure.
LPstep or QPstep	is the step length α taken along the current search direction p. The variables x have just been changed to $x + \alpha p$. Write Step to stand for LPStep or QPStep, depending on the problem. If a variable is made superbasic during the current iteration (+SBS > 0), Step will be the step to the nearest bound. During the solution of (11), the step can be greater than one only if the reduced Hessian is not positive definite.
nInf	is the number of infeasibilities *after* the present iteration. This number will not increase unless the iterations are in elastic mode.

`SumInf` is the sum of infeasibilities after the present iteration, if `nInf` > 0. The value usually decreases at each nonzero `Step`, but if it decreases by 2 or more, `SumInf` may occasionally increase.

`rgNorm` is the norm of the reduced-gradient vector at the start of the iteration. (It is the norm of the vector with elements d_j for variables j in the superbasic set.) During the solution of subproblem (11) this norm will be approximately zero after a unit step. (The heading is not printed if the problem is linear.)

`LPobjective`, `QPobjective` or `Elastic QPobj`
the QP objective function after the present iteration. In elastic mode, the heading is changed to `Elastic QPobj`. In either case, the value printed decreases monotonically.

`+SBS` is the variable `jq` selected by the pricing operation to be added to the superbasic set.

`-SBS` is the superbasic variable chosen to become nonbasic.

`-BS` is the basis variable removed (if any) to become nonbasic.

`Pivot` if column a_q replaces the rth column of the basis B, `Pivot` is the rth element of a vector y satisfying $By = a_q$. Wherever possible, `Step` is chosen to avoid extremely small values of `Pivot` (since they cause the basis to be nearly singular). In rare cases, it may be necessary to increase the **Pivot Tolerance** to exclude very small elements of y from consideration during the computation of `Step`.

`L+U` is the number of nonzeros representing the basis factors L and U. Immediately after a basis factorization $B = LU$, `L+U` is `lenL+lenU`, the number of subdiagonal elements in the columns of a lower triangular matrix and the number of diagonal and superdiagonal elements in the rows of an upper-triangular matrix. Further nonzeros are added to `L` when various columns of B are later replaced. As columns of B are replaced, the matrix U is maintained explicitly (in sparse form). The value of `L` will steadily increase, whereas the value of `U` may fluctuate up or down. Thus the value of `L+U` may fluctuate up or down (in general, it will tend to increase).

`ncp` is the number of compressions required to recover storage in the data structure for U. This includes the number of compressions needed during the previous basis factorization.

`nS` is the current number of superbasic variables. (The heading is not printed if the problem is linear.)

`condHz` see Section 13.1. (The heading is not printed if the problem is linear.)

13.3 Crash Statistics

If **Major Print Level** ≥ 10 and **System Information Yes** has been specified, the following items are output to the Print file when **Cold Start** and no Backup Basis file is loaded. They refer to the number of columns that the Crash procedure selects during selected passes through A while searching for a triangular basis matrix.

Label	**Description**
`Slacks`	is the number of slacks selected initially.
`Free cols`	is the number of free columns in the basis.
`Preferred`	is the number of 'preferred' columns in the basis (i.e., **istate**$[j-1] = 3$ for some $j \leq n$).

`Unit` is the number of unit columns in the basis.

`Double` is the number of columns in the basis containing 2 nonzeros.

`Triangle` is the number of triangular columns in the basis.

`Pad` is the number of slacks used to pad the basis (to make it a nonsingular triangle).

13.4 Basis Factorization Statistics

If **Major Print Level** ≥ 10, the first seven items in the list below are output to the Print file whenever the basis B or the rectangular matrix $B_S = \begin{pmatrix} B & S \end{pmatrix}^{\mathrm{T}}$ is factorized before solution of the next QP subproblem. See Section 12.1 for a full description of an optional argument.

Gaussian elimination is used to compute a sparse LU factorization of B or B_S, where PLP^{T} and PUQ are lower and upper triangular matrices for some permutation matrices P and Q. Stability is ensured as described under the optional argument **LU Factor Tolerance**.

If **Minor Print Level** ≥ 10, the same items are printed during the QP solution whenever the current B is factorized. In addition, if **System Information Yes** has been specified, the entries from `Elems` onwards are also printed.

Label **Description**

`Factor` the number of factorizations since the start of the run.

`Demand` a code giving the reason for the present factorization, as follows:

Code	Meaning
0	First LU factorization.
1	The number of updates reached the **Factorization Frequency**.
2	The nonzeros in the updated factors have increased significantly.
7	Not enough storage to update factors.
10	Row residuals too large (see the description of the optional argument **Check Frequency**).
11	Ill-conditioning has caused inconsistent results.

`Itn` is the current minor iteration number.

`Nonlin` is the number of nonlinear variables in the current basis B.

`Linear` is the number of linear variables in B.

`Slacks` is the number of slack variables in B.

`B BR BS or BT factorize`
is the type of LU factorization.

`B`	periodic factorization of the basis B.
`BR`	more careful rank-revealing factorization of B using threshold rook pivoting. This occurs mainly at the start, if the first basis factors seem singular or ill-conditioned. Followed by a normal `B` factorize.
`BS`	B_S is factorized to choose a well-conditioned B from the current $(B\ S)$. Followed by a normal `B` factorize.
`BT`	same as `BS` except the current B is tried first and accepted if it appears to be not much more ill-conditioned than after the previous `BS` factorize.

`m` is the number of rows in B or B_S.

`n` is the number of columns in B or B_S. Preceded by '=' or '>' respectively.

`Elems` is the number of nonzero elements in B or B_S.

`Amax` is the largest nonzero in B or B_S.

`Density` is the percentage nonzero density of B or B_S.

`Merit/MerRP/MerCP` is the average Markowitz merit count for the elements chosen to be the diagonals of PUQ. Each merit count is defined to be $(c-1)(r-1)$ where c and r are the number of nonzeros in the column and row containing the element at the time it is selected to be the next diagonal. `Merit` is the average of `n` such quantities. It gives an indication of how much work was required to preserve sparsity during the factorization. If **LU Complete Pivoting** or **LU Rook Pivoting** has been selected, this heading is changed to `MerCP`, respectively `MerRP`.

`lenL` is the number of nonzeros in L.

`L+U` is the number of nonzeros representing the basis factors L and U. Immediately after a basis factorization $B = LU$, `L+U` is `lenL+lenU`, the number of subdiagonal elements in the columns of a lower triangular matrix and the number of diagonal and superdiagonal elements in the rows of an upper-triangular matrix. Further nonzeros are added to `L` when various columns of B are later replaced. As columns of B are replaced, the matrix U is maintained explicitly (in sparse form). The value of `L` will steadily increase, whereas the value of `U` may fluctuate up or down. Thus the value of `L+U` may fluctuate up or down (in general, it will tend to increase).

`Cmpressns` is the number of times the data structure holding the partially factored matrix needed to be compressed to recover unused storage. Ideally this number should be zero. If it is more than 3 or 4, the amount of workspace available to nag_opt_nlp_solve (e04wdc) should be increased for efficiency.

`Incres` is the percentage increase in the number of nonzeros in L and U relative to the number of nonzeros in B or B_S.

`Utri` is the number of triangular rows of B or B_S at the top of U.

`lenU` the number of nonzeros in U, including its diagonals.

`Ltol` is the largest subdiagonal element allowed in L. This is the specified **LU Factor Tolerance** or a smaller value that is currently being used for greater stability.

`Umax` the maximum nonzero element in U.

`Ugrwth` is the ratio `Umax`/`Amax`, which ideally should not be substantially larger than 10.0 or 100.0. If it is orders of magnitude larger, it may be advisable to reduce the **LU Factor Tolerance** to 5.0, 4.0, 3.0 or 2.0, say (but bigger than 1.0).

As long as `Lmax` is not large (say 5.0 or less), $\max(\texttt{Amax}, \texttt{Umax})/\texttt{DUmin}$ gives an estimate of the condition number B. If this is extremely large, the basis is nearly singular. Slacks are used to replace suspect columns of B and the modified basis is refactored.

`Ltri` is the number of triangular columns of B or B_S at the left of L.

`dense1` is the number of columns remaining when the density of the basis matrix being factorized reached 0.3.

`Lmax` is the actual maximum subdiagonal element in L (bounded by `Ltol`).

`Akmax` is the largest nonzero generated at any stage of the LU factorization. (Values much larger than `Amax` indicate instability.) `Akmax` is not printed if **LU Partial Pivoting** is selected.

`Agrwth` is the ratio `Akmax`/`Amax`. Values much larger than 100 (say) indicate instability. Growth is not printed if **LU Partial Pivoting** is selected.

`bump` is the size of the block to be factorized nontrivially after the triangular rows and columns of B or B_S have been removed.

`dense2` is the number of columns remaining when the density of the basis matrix being factorized reached 0.6. (The Markowitz pivot strategy searches fewer columns at that stage.)

`DUmax` is the largest diagonal of PUQ.

`DUmin` is the smallest diagonal of PUQ.

`condU` the ratio `DUmax`/`DUmin`, which estimates the condition number of U (and of B if `Ltol` is less than 5.0, say).

13.5 The Solution File

At the end of a run, the final solution may be output as a Solution file, according to **Solution File**. Some header information appears first to identify the problem and the final state of the optimization procedure. A ROWS section and a COLUMNS section then follow, giving one line of information for each row and column. The format used is similar to certain commercial systems, though there is no industry standard.

The maximum record length is 111 characters.

To reduce clutter, a full stop (.) is printed for any numerical value that is exactly zero. The values ± 1 are also printed specially as 1.0 and -1.0. Infinite bounds ($\pm 10^{20}$ or larger) are printed as `None`.

A Solution file is intended to be read from disk by a self-contained program that extracts and saves certain values as required for possible further computation. Typically, the first 14 records would be ignored. Each subsequent record may be read . The end of the ROWS section is marked by a record that starts with a 1 and is otherwise blank. If this and the next 4 records are skipped, the COLUMNS section can then be read under the same format.

13.5.1 The ROWS section

General linear constraints take the form $l \leq Ax \leq u$. The ith constraint is therefore of the form

$$\alpha \leq \nu_i x \leq \beta,$$

where ν_i is the ith row of A.

Internally, the constraints take the form $Ax - s = 0$, where s is the set of slack variables (which happen to satisfy the bounds $l \leq s \leq u$). For the ith constraint it is the slack variable s_i that is directly available, and it is sometimes convenient to refer to its state. Nonlinear constraints $\alpha \leq c_i(x) + v_i x \leq \beta$ are treated similarly, except that the row activity and degree of infeasibility are computed directly from $c_i(x) + v_i x$ rather than s_i. A fullstop (.) is printed for any numerical value that is exactly zero.

Label **Description**

`Number` is the value of $n + i$. (This is used internally to refer to s_i in the intermediate output.)

`Row` gives the name of the ith row.

`State` the state of the ith row relative to the bounds α and β. The various states possible are as follows:

- `LL` the row is at its lower limit, α.
- `UL` the row is at its upper limit, β.
- `EQ` the limits are the same ($\alpha = \beta$).
- `FR` s_i is nonbasic and currently zero, even though it is free to take any value between its bounds α and β.
- `BS` s_i is basic.
- `SBS` s_i is superbasic.

A key is sometimes printed before `State`. Note that unless the optional argument **Scale Option** $= 0$ is specified, the tests for assigning a key are applied to the variables of the scaled problem.

- `A` *Alternative optimum possible*. The variable is nonbasic, but its reduced gradient is essentially zero. This means that if the variable were allowed to start moving away from its bound, there would be no change in the value of

the objective function. The values of the other free variables *might* change, giving a genuine alternative solution. However, if there are any degenerate variables (labelled `D`), the actual change might prove to be zero, since one of them could encounter a bound immediately. In either case, the values of the Lagrange multipliers *might* also change.

`D` *Degenerate*. The variable is basic or superbasic, but it is equal (or very close) to one of its bounds.

`I` *Infeasible*. The variable is basic or superbasic and is currently violating one of its bounds by more than the value of the **Feasibility Tolerance**.

`N` *Not precisely optimal*. The variable is nonbasic or superbasic. If the value of the reduced gradient for the variable exceeds the value of the optional argument **Major Optimality Tolerance**, the solution would not be declared optimal because the reduced gradient for the variable would not be considered negligible.

`Activity` is the value of $v_i x$ (or $c_i(x) + v_i x$ for nonlinear rows) at the final iterate.

`Slack Activity` is the value by which the row differs from its nearest bound. (For the free row (if any), it is set to `Activity`.)

`Lower Limit` is α, the lower bound on the row.

`Upper Limit` is β, the upper bound on the row.

`Dual Activity` is the value of the dual variable π_i (the Lagrange multiplier for the ith constraint). The full vector π always satisfies $B^{\mathrm{T}}\pi = g_B$, where B is the current basis matrix and g_B contains the associated gradients for the current objective function. For FP problems, π_i is set to zero.

`i` gives the index i of the ith row.

13.5.2 The COLUMNS section

Let the jth component of x be the variable x_j and assume that it satisfies the bounds $\alpha \leq x_j \leq \beta$. A fullstop (.) is printed for any numerical value that is exactly zero.

Label	**Description**
`Number`	is the column number j. (This is used internally to refer to x_j in the intermediate output.)
`Column`	gives the name of x_j.
`State`	the state of x_j relative to the bounds α and β. The various states possible are as follows:

`LL` x_j is nonbasic at its lower limit, α.

`UL` x_j is nonbasic at its upper limit, β.

`EQ` x_j is nonbasic and fixed at the value $\alpha = \beta$.

`FR` x_j is nonbasic at some value strictly between its bounds: $\alpha < x_j < \beta$.

`BS` x_j is basic. Usually $\alpha < x_j < \beta$.

`SBS` x_j is superbasic. Usually $\alpha < x_j < \beta$.

A key is sometimes printed before `State`. Note that unless the optional argument **Scale Option** $= 0$ is specified, the tests for assigning a key are applied to the variables of the scaled problem.

`A` *Alternative optimum possible*. The variable is nonbasic, but its reduced gradient is essentially zero. This means that if the variable were allowed to start moving away from its bound, there would be no change in the value of the objective function. The values of the other free variables *might* change,

giving a genuine alternative solution. However, if there are any degenerate variables (labelled `D`), the actual change might prove to be zero, since one of them could encounter a bound immediately. In either case, the values of the Lagrange multipliers *might* also change.

`D` *Degenerate*. The variable is basic or superbasic, but it is equal (or very close) to one of its bounds.

`I` *Infeasible*. The variable is basic or superbasic and is currently violating one of its bounds by more than the value of the **Feasibility Tolerance**.

`N` *Not precisely optimal*. The variable is nonbasic or superbasic. If the value of the reduced gradient for the variable exceeds the value of the optional argument **Major Optimality Tolerance**, the solution would not be declared optimal because the reduced gradient for the variable would not be considered negligible.

`Activity` is the value of x_j at the final iterate.

`Obj Gradient` is the value of g_j at the final iterate. For FP problems, g_j is set to zero.

`Lower Limit` is the lower bound specified for the variable. `None` indicates that $\mathbf{bl}[j-1] \leq -bigbnd$.

`Upper Limit` is the upper bound specified for the variable. `None` indicates that $\mathbf{bu}[j-1] \geq bigbnd$.

`Reduced Gradnt` is the value of the reduced gradient $d_j = g_j - \pi^{\mathrm{T}} a_j$ where a_j is the jth column of the constraint matrix. For FP problems, d_j is set to zero.

`m + j` is the value of $m + j$.

Note that movement off a constraint (as opposed to a variable moving away from its bound) can be interpreted as allowing the entry in the `Slack Activity` column to become positive.

Numerical values are output with a fixed number of digits; they are not guaranteed to be accurate to this precision.

13.6 The Summary File

If **Summary File** > 0, the following information is output to the **Summary File**. (It is a brief summary of the output directed to unit **Print File**):

– the optional arguments supplied via the option setting functions, if any;

– the Basis file loaded, if any;

– a brief major iteration log (see Section 13.1);

– a brief minor iteration log (see Section 13.2);

– the exit condition, **fail**;

– a summary of the final iterate.