NAG Library Function Document

nag_opt_nlp_sparse (e04ugc)

1 Purpose

nag_opt_nlp_sparse (e04ugc) solves sparse nonlinear programming problems.

2 Specification

```
#include <nag.h>
#include <nage04.h>
void nag_opt_nlp_sparse (
     void (*confun)(Integer ncnln, Integer njnln, Integer nnzjac,
          const double x[], double conf[], double conjac[], Nag_Comm *comm),
     void (*objfun)(Integer nonln, const double x[], double *objf,
          double objgrad[], Nag_Comm *comm),
     Integer n, Integer m, Integer ncnln, Integer nonln, Integer njnln,
     Integer iobj, Integer nnz, double a[], const Integer ha[],
     const Integer ka[], double bl[], double bu[], double xs[],
     Integer *ninf, double *sinf, double *objf, Nag_Comm *comm,
     Nag_E04_Opt *options, NagError *fail)
```

3 Description

nag_opt_nlp_sparse (e04ugc) is designed to solve a class of nonlinear programming problems that are assumed to be stated in the following general form:

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

where $x = (x_1, x_2, \ldots, x_n)^{\mathrm{T}}$ is a set of variables, $f(x)$ is a smooth scalar objective function, l and u are constant lower and upper bounds, $F(x)$ is a vector of smooth nonlinear constraint functions $\{F_i(x)\}$ and G is a *sparse* matrix.

The constraints involving F and Gx are called the *general constraints*. Note that upper and lower bounds are specified for all variables and constraints. This form allows full generality in specifying various types of constraint. In particular, the jth constraint can be defined as an *equality* by setting $l_j = u_j$. 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 parameter **options**.**inf_bound** in Section 12.2).

nag_opt_nlp_sparse (e04ugc) converts the upper and lower bounds on the m elements of F and Gx to equalities by introducing a set of *slack variables* s, where $s = (s_1, s_2, \ldots, s_m)^{\mathrm{T}}$. 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 problem defined by (1) can therefore be re-written in the following equivalent form:

$$\underset{x\in R^n, s\in R^m}{\text{minimize}} f(x) \quad \text{subject to} \quad \begin{Bmatrix} F(x) \\ Gx \end{Bmatrix} - s = 0, \quad l \leq \begin{Bmatrix} x \\ s \end{Bmatrix} \leq u. \tag{2}$$

Since the slack variables s are subject to the same upper and lower bounds as the elements of F and Gx, the bounds on F and Gx can simply be thought of as bounds on the combined vector (x, s). The elements of x and s are partitioned into *basic*, *nonbasic* and *superbasic variables* defined as follows (see Section 11 for more details):

A *basic* variable is a variable associated with a column of a square nonsingular basis matrix B.

A *nonbasic* variable is a variable that is temporarily fixed at its current value (usually its upper or lower bound).

A *superbasic* variable is a non basic variable which is not at one of its bounds and which is free to move in any desired direction (namely one that will improve the value of the objective function or reduce the sum of infeasibilities). At each step, basic variables are adjusted depending on the values of superbasic variables.

For example, in the simplex method (see Gill *et al.* (1981)) the elements of x can be partitioned at each vertex into a set of m basic variables (all non-negative) and a set of $(n-m)$ nonbasic variables (all zero). This is equivalent to partitioning the columns of the constraint matrix as $(B \mid N)$, where B contains the m columns that correspond to the basic variables and N contains the $(n-m)$ columns that correspond to the nonbasic variables.

The optional parameter **options.direction** (default value **options.direction** = Nag_Minimize) may be used to specify an alternative problem in which $f(x)$ is maximized (setting **options.direction** = Nag_Maximize), or to only find a feasible point (setting **options.direction** = Nag_FeasiblePoint). If the objective function is nonlinear and all the constraints are linear, F is absent and the problem is said to be *linearly constrained*. In general, the objective and constraint functions are *structured* in the sense that they are formed from sums of linear and nonlinear functions. This structure can be exploited by the function during the solution process as follows.

Consider the following nonlinear optimization problem with four variables (u, v, z, w):

$$\underset{u,v,z,w}{\text{minimize}} (u+v+z)^2 + 3z + 5w$$

subject to the constraints

$$\begin{aligned} u^2 + v^2 + z &= 2 \\ u^4 + v^4 + w &= 4 \\ 2u + 4v &\geq 0 \end{aligned}$$

and to the bounds

$$\begin{aligned} z &\geq 0 \\ w &\geq 0 \end{aligned}.$$

This problem has several characteristics that can be exploited by the function:

the objective function is nonlinear. It is the sum of a *nonlinear* function of the variables (u, v, z) and a *linear* function of the variables (z, w);

the first two constraints are nonlinear. The third is linear;

each nonlinear constraint function is the sum of a *nonlinear* function of the variables (u, v) and a *linear* function of the variables (z, w).

The nonlinear terms are defined by the user-supplied subroutines **objfun** and **confun** (see Section 5), which involve only the appropriate subset of variables.

For the objective, we define the function $f(u, v, z) = (u+v+z)^2$ to include only the nonlinear part of the objective. The three variables (u, v, z) associated with this function are known as the *nonlinear objective variables*. The number of them is given by **nonln** (see Section 5), and they are the only variables needed in **objfun**. The linear part $3z + 5w$ of the objective is stored in row **iobj** (see Section 5) of the (constraint) Jacobian matrix A (see below).

Thus, if x' and y' denote the nonlinear and linear objective variables, respectively, the objective may be re-written in the form

$$f(x') + c^{\mathrm{T}} x' + d^{\mathrm{T}} y',$$

where $f(x')$ is the nonlinear part of the objective and c and d are constant vectors that form a row of A. In this example, $x' = (u, v, z)$ and $y' = w$.

Similarly for the constraints, we define a vector function $F(u,v)$ to include just the nonlinear terms. In this example, $F_1(u,v) = u^2 + v^2$ and $F_2(u,v) = u^4 + v^4$, where the two variables (u,v) are known as the *nonlinear Jacobian variables*. The number of them is given by **njnln** (see Section 5), and they are the only variables needed in **confun**. Thus, if x'' and y'' denote the nonlinear and linear Jacobian variables, respectively, the constraint functions and the linear part of the objective have the form

$$\begin{pmatrix} F(x'') & A_2y'' \\ A_3x'' & A_4y'' \end{pmatrix}, \tag{3}$$

where $x'' = (u,v)$ and $y'' = (z,w)$ in this example. This ensures that the Jacobian is of the form

$$A = \begin{pmatrix} J(x'') & A_2 \\ A_3 & A_4 \end{pmatrix}$$

where $J(x'') = \dfrac{\partial F(x'')}{\partial x}$. Note that $J(x'')$ *always* appears in the *top left-hand corner* of A.

The inequalities $l_1 \leq F(x'') + A_2y'' \leq u_1$ and $l_2 \leq A_3x'' + A_4y'' \leq u_2$ implied by the constraint functions in (3) are known as the *nonlinear* and *linear* constraints, respectively. The nonlinear constraint vector $F(x'')$ in (3) and (optionally) its partial derivative matrix $J(x'')$ are set in **confun**. The matrices A_2, A_3 and A_4 contain any (constant) linear terms. Along with the sparsity pattern of $J(x'')$ they are stored in the arrays **a**, **ha** and **ka** (see Section 5).

In general, the vectors x' and x'' have different dimensions, but they *must* always overlap, in the sense that the shorter vector should always be the beginning of the other. In the above example, the nonlinear Jacobian variables (u,v) are an ordered subset of the nonlinear objective variables (u,v,z). In other cases it could be the other way round. Note that in some cases it might be necessary to add variables to x' or x'' (whichever is the most convenient), but the first way keeps $J(x'')$ as small as possible. Thus, the nonlinear objective function $f(x')$ may involve either a subset or superset of the variables appearing in the nonlinear constraint functions $F(x'')$, and **nonln** $\leq$ **njnln** (or vice-versa). Sometimes the objective and constraints may really involve *disjoint sets of nonlinear variables*. In such cases the variables should be ordered so that **nonln** $>$ **njnln** and $x' = (x'', x''')$, where the objective is nonlinear in just the last vector x'''. The first **njnln** elements of the gradient array **objgrad** (corresponding to x'') should then be set to zero in **objfun**. This is illustrated in Section 10.

If there are no nonlinear constraints in (1) and $f(x)$ is linear or quadratic, then it may be simpler and/or more efficient to use nag_opt_sparse_convex_qp (e04nkc) to solve the resulting linear or quadratic programming problem, or one of nag_opt_lp (e04mfc), nag_opt_lin_lsq (e04ncc) or nag_opt_qp (e04nfc) if G is a *dense* matrix. If the problem is dense and does have nonlinear constraints, then nag_opt_nlp (e04ucc) should be used instead.

You must supply an initial estimate of the solution to (1), together with versions of **objfun** and **confun** that define $f(x')$ and $F(x'')$, respectively, and as many first partial derivatives as possible. Note that if there are any nonlinear constraints, then the *first* call to **confun** will precede the *first* call to **objfun**.

nag_opt_nlp_sparse (e04ugc) is based on the SNOPT package described in Gill *et al.* (1997), which in turn utilizes routines from the MINOS package (see Murtagh and Saunders (1995)). It incorporates a sequential quadratic programming (SQP) method that obtains search directions from a sequence of quadratic programming (QP) subproblems. Each QP subproblem minimizes a quadratic model of a certain Lagrangian function subject to a linearization of the constraints. An augmented Lagrangian merit function is reduced along each search direction to ensure convergence from any starting point. Further details can be found in Section 11.

Throughout this document the symbol ϵ is used to represent the ***machine precision*** (see nag_machine_precision (X02AJC)).

4 References

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5 Arguments

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

confun must calculate the vector $F(x)$ of nonlinear constraint functions and (optionally) its Jacobian $(=\dfrac{\partial F}{\partial x})$ for a specified **njnln** $(\leq n)$ element vector x. If there are no nonlinear constraints (i.e., **ncnln** $= 0$), **confun** will never be called by nag_opt_nlp_sparse (e04ugc) and the NAG defined null void function pointer, `NULLFN`, can be supplied in the call to nag_opt_nlp_sparse (e04ugc). If there are nonlinear constraints, the first call to **confun** will occur before the first call to **objfun**.

The specification of **confun** is:

```
void confun (Integer ncnln, Integer njnln, Integer nnzjac,
     const double x[], double conf[], double conjac[], Nag_Comm *comm)
```

1: **ncnln** – Integer *Input*

On entry: the number of nonlinear constraints. These must be the first **ncnln** constraints in the problem.

2: **njnln** – Integer *Input*

On entry: the number of nonlinear variables. These must be the first **njnln** variables in the problem.

3: **nnzjac** – Integer *Input*

On entry: the number of nonzero elements in the constraint Jacobian. Note that **nnzjac** will always be less than, or equal to, **ncnln** × **njnln**.

4: **x**[**njnln**] – const double *Input*

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

5: **conf**[**ncnln**] – double *Output*

On exit: if **comm**→**flag** $= 0$ or 2, **conf**$[i-1]$ must contain the value of $F_i(x)$, the ith nonlinear constraint at x.

6: **conjac**[**nnzjac**] – double *Output*

On exit: if **comm**→**flag** $= 1$ or 2, **conjac** must return the available elements of $J(x)$, the constraint Jacobian evaluated at x. These elements must be stored in **conjac** in exactly the same positions as implied by the definitions of the arrays **a**, **ha** and **ka** described below, remembering that $J(x)$ always appears in the top left-hand corner of A. Note that the function does not perform any internal checks for consistency (except indirectly via the optional parameter **options**.**verify_grad**), so great care is essential.

If all elements of the constraint Jacobian are known, i.e., the optional parameter **options**.**con_deriv** = Nag_TRUE (the default), any constant elements of the Jacobian may be assigned to **a** at the start of the optimization if desired. If an element of **conjac** is not assigned in **confun**, the corresponding value from **a** is used. See also the description for **a**.

If **options**.**con_deriv** = Nag_FALSE, then any available partial derivatives of $c_i(x)$ must be assigned to the elements of **conjac**; the remaining elements *must remain unchanged*. It must be emphasized that, in that case, unassigned elements of **conjac** are not treated as constant; they are estimated by finite differences, at non-trivial expense.

7: **comm** – Nag_Comm *

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

flag – Integer *Input/Output*

On entry: **confun** is called with **comm**→**flag** set to 0, 1 or 2.

If **comm**→**flag** $= 0$, only **conf** has to be referenced.

If **comm**→**flag** $= 1$, only **conjac** has to be referenced.

If **comm**→**flag** $= 2$, both **conf** and **conjac** are referenced.

On exit: if **confun** resets **comm**→**flag** to -1, nag_opt_nlp_sparse (e04ugc) will terminate with the error indicator NE_CANNOT_CALCULATE, unless this occurs during the linesearch; in this case, the linesearch will shorten the step and try again. If **confun** resets **comm**→**flag** to a value smaller or equal to -2,, nag_opt_nlp_sparse (e04ugc) will terminate immediately with the error indicator NE_USER_STOP. In both cases, if **fail** is supplied to nag_opt_nlp_sparse (e04ugc), **fail**.**errnum** will be set to your setting of **comm**→**flag**.

first – Nag_Boolean *Input*

On entry: will be set to Nag_TRUE on the first call to **confun** and Nag_FALSE for all subsequent calls. This argument setting allows you to save computation time if certain data must be read or calculated only once.

last – Nag_Boolean *Input*

On entry: will be set to Nag_TRUE on the last call to **confun** and Nag_FALSE for all other calls. This argument setting allows you to perform some additional computation on the final solution.

user – double *
iuser – Integer *
p – Pointer

The type Pointer is `void *`.

Before calling nag_opt_nlp_sparse (e04ugc) these pointers may be allocated memory and initialized with various quantities for use by **confun** when called from nag_opt_nlp_sparse (e04ugc).

Note: **confun** should be tested separately before being used in conjunction with nag_opt_nlp_sparse (e04ugc). The optional parameters **options**.**verify_grad** and **options**.**major_iter_lim** can be used to assist this process (see Section 12.2). The array **x** must **not** be changed by **confun**.

If **confun** does not calculate all of the Jacobian constraint elements then the optional parameter **options**.**con_deriv** should be set to Nag_FALSE.

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

objfun must calculate the nonlinear part of the objective $f(x)$ and (optionally) its gradient $(= \dfrac{\partial f}{\partial x})$ for a specified **nonln** $(\leq \mathbf{n})$ element vector x. If there are no nonlinear objective variables (i.e., **nonln** $= 0$), **objfun** will never be called by nag_opt_nlp_sparse (e04ugc) and the NAG defined null void function pointer, `NULLFN`, can be supplied in the call to nag_opt_nlp_sparse (e04ugc).

The specification of **objfun** is:

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

1: **nonln** – Integer *Input*

On entry: the number of nonlinear objective variables. These must be the first **nonln** variables in the problem.

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

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

3: **objf** – double * *Output*

On exit: if **comm**→**flag** $= 0$ or 2, **objfun** must set **objf** to the value of the nonlinear part of the objective function at x. If it is not possible to evaluate the objective function at x, then **objfun** should assign -1 to **comm**→**flag**; nag_opt_nlp_sparse (e04ugc) will then terminate, unless this occurs during the linesearch; in this case, the linesearch will shorten the step and try again.

4: **objgrad**[**nonln**] – double *Output*

On exit: if **comm**→**flag** $= 1$ or 2, **objgrad** must return the available elements of the gradient $\dfrac{\partial f}{\partial x}$ evaluated at the current point x.

If the optional parameter **options**.**obj_deriv** = Nag_TRUE (the default), all elements of **objgrad** must be set; if **options**.**obj_deriv** = Nag_FALSE, any available elements of the

Jacobian matrix must be assigned to the elements of **objgrad**; the remaining elements *must remain unchanged*.

5: **comm** – Nag_Comm *

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

flag – Integer *Input/Output*

On entry: **objfun** is called with **comm**→**flag** set to 0, 1 or 2.

If **comm**→**flag** = 0 then only **objf** has to be referenced.

If **comm**→**flag** = 1 then only **objgrad** has to be referenced.

If **comm**→**flag** = 2 then both **objf** and **objgrad** are referenced.

On exit: if **objfun** resets **comm**→**flag** to −1, then nag_opt_nlp_sparse (e04ugc) will terminate with the error indicator NE_CANNOT_CALCULATE, unless this occurs during the linesearch; in this case, the linesearch will shorten the step and try again. If **objfun** resets **comm**→**flag** to a value smaller or equal to −2, then nag_opt_nlp_sparse (e04ugc) will terminate immediately with the error indicator NE_USER_STOP. In both cases, if **fail** is supplied to nag_opt_nlp_sparse (e04ugc) **fail**.**errnum** will then be set to your setting of **comm**→**flag**.

first – Nag_Boolean *Input*

On entry: will be set to Nag_TRUE on the first call to **objfun** and Nag_FALSE for all subsequent calls. This argument setting allows you to save computation time if certain data must be read or calculated only once.

last – Nag_Boolean *Input*

On entry: will be set to Nag_TRUE on the last call to **objfun** and Nag_FALSE for all other calls. This argument setting allows you to perform some additional computation on the final solution.

nf – Integer *Input*

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

user – double *
iuser – Integer *
p – Pointer

The type Pointer is `void *`.

Before calling nag_opt_nlp_sparse (e04ugc) these pointers may be allocated memory and initialized with various quantities for use by **objfun** when called from nag_opt_nlp_sparse (e04ugc).

Note: **objfun** should be tested separately before being used in conjunction with nag_opt_nlp_sparse (e04ugc). The optional parameters **options**.**verify_grad** and **options**.**major_iter_lim** can be used to assist this process (see Section 12.2). The array **x** must **not** be changed by **objfun**.

If the function **objfun** does not calculate all of the Jacobian elements then the optional parameter **options**.**obj_deriv** should be set to Nag_FALSE.

3: **n** – Integer *Input*

On entry: n, the number of variables (excluding slacks). This is the number of columns in the full Jacobian matrix A.

Constraint: **n** ≥ 1.

4: **m** – Integer *Input*

On entry: m, the number of general constraints (or slacks). This is the number of rows in A, including the free row (if any; see **iobj**). Note that A must contain at least one row. If your problem has no constraints, or only upper and lower bounds on the variables, then you must include a dummy 'free' row consisting of a single (zero) element subject to 'infinite' upper and lower bounds. Further details can be found under the descriptions for **iobj**, **nnz**, **a**, **ha**, **ka**, **bl** and **bu**.

Constraint: $\mathbf{m} \geq 1$.

5: **ncnln** – Integer *Input*

On entry: the number of nonlinear constraints. These correspond to the leading **ncnln** rows of A.

Constraint: $0 \leq \mathbf{ncnln} \leq \mathbf{m}$.

6: **nonln** – Integer *Input*

On entry: the number of nonlinear objective variables. If the objective function is nonlinear, the leading **nonln** columns of A belong to the nonlinear objective variables. (See also the description for **njnln**.)

Constraint: $0 \leq \mathbf{nonln} \leq \mathbf{n}$.

7: **njnln** – Integer *Input*

On entry: the number of nonlinear Jacobian variables. If there are any nonlinear constraints, the leading **njnln** columns of A belong to the nonlinear Jacobian variables. If $\mathbf{nonln} > 0$ and $\mathbf{njnln} > 0$, the nonlinear objective and Jacobian variables overlap. The total number of nonlinear variables is given by $\bar{n} = \max(\mathbf{nonln}, \mathbf{njnln})$.

Constraints:

if $\mathbf{ncnln} = 0$, $\mathbf{njnln} = 0$;
if $\mathbf{ncnln} > 0$, $1 \leq \mathbf{njnln} \leq \mathbf{n}$.

8: **iobj** – Integer *Input*

On entry: if $\mathbf{iobj} > \mathbf{ncnln}$, row **iobj** of A is a free row containing the nonzero elements of the linear part of the objective function.

$\mathbf{iobj} = 0$
There is no free row.

$\mathbf{iobj} = -1$
There is a dummy 'free' row.

Constraints:

if $\mathbf{iobj} > 0$, $\mathbf{ncnln} < \mathbf{iobj} \leq \mathbf{m}$;
otherwise $\mathbf{iobj} \geq -1$.

9: **nnz** – Integer *Input*

On entry: the number of nonzero elements in A (including the Jacobian for any nonlinear constraints, J). If $\mathbf{iobj} = -1$, set $\mathbf{nnz} = 1$.

Constraint: $1 \leq \mathbf{nnz} \leq \mathbf{n} \times \mathbf{m}$.

10: **a**[**nnz**] – double *Input/Output*

On entry: the nonzero elements of the Jacobian matrix A, ordered by increasing column index. Note that elements with the same row and column index are not allowed. Since the constraint Jacobian matrix $J(x'')$ must always appear in the top left-hand corner of A, those elements in a column associated with any nonlinear constraints must come before any elements belonging to the linear constraint matrix G and the free row (if any; see **iobj**).

In general, A is partitioned into a nonlinear part and a linear part corresponding to the nonlinear variables and linear variables in the problem. Elements in the nonlinear part may be set to any value (e.g., zero) because they are initialized at the first point that satisfies the linear constraints and the upper and lower bounds. If the optional parameter **options.con_deriv** = Nag_TRUE (the default), the nonlinear part may also be used to store any constant Jacobian elements. Note that if **confun** does not define the constant Jacobian element **conjac**$[i]$, the missing value will be obtained directly from the corresponding element of **a**. The linear part must contain the nonzero elements of G and the free row (if any). If **iobj** $= -1$, set **a**$[0] = \beta$, say, where $|\beta| < bigbnd$ and $bigbnd$ is the value of the optional parameter **options.inf_bound** (default value $= 10^{20}$). Elements with the same row and column indices are not allowed. (See also the descriptions for **ha** and **ka**.)

On exit: elements in the nonlinear part corresponding to nonlinear Jacobian variables are overwritten.

11: **ha**[**nnz**] – const Integer *Input*

On entry: **ha**$[i-1]$ must contain the row index of the nonzero element stored in **a**$[i-1]$, for $i = 1, 2, \ldots,$ **nnz**. The row indices for a column may be supplied in any order subject to the condition that those elements in a column associated with any nonlinear constraints must appear before those elements associated with any linear constraints (including the free row, if any). Note that **confun** must define the Jacobian elements in the same order. If **iobj** $= -1$, set **ha**$[0] = 1$.

Constraint: $1 \leq$ **ha**$[i-1] \leq$ **m**, for $i = 1, 2, \ldots,$ **nnz**.

12: **ka**[**n** + **1**] – const Integer *Input*

On entry: **ka**$[j-1]$ must contain the index in **a** of the start of the jth column, for $j = 1, 2, \ldots,$ **n**. To specify the jth column as empty, set **ka**$[j]$ = **ka**$[j-1]$. Note that the first and last elements of **ka** must be such that **ka**$[0] = 0$ and **ka**[**n**] = **nnz**. If **iobj** $= -1$, set **ka**$[j] = 1$, for $j = 1, 2, \ldots,$ **n**.

Constraints:

ka$[0] = 0$;
ka$[j-1] \geq 0$, for $j = 2, 3, \ldots,$ **n**;
ka[**n**] = **nnz**;
$0 \leq$ **ka**$[j]$ − **ka**$[j-1] \leq$ **m**, for $j = 1, 2, \ldots,$ **n**.

13: **bl**[**n** + **m**] – double *Input/Output*
14: **bu**[**n** + **m**] – double *Input/Output*

On entry: **bl** must contain the lower bounds l and **bu** the upper bounds u, for all the variables and general constraints, in the following order. The first **n** elements of **bl** must contain the bounds on the variables **x**, the next **ncnln** elements the bounds for the nonlinear constraints $F(x)$ (if any) and the next (**m** − **ncnln**) elements the bounds for the linear constraints Gx and the free row (if any). To specify a nonexistent lower bound (i.e., $l_j = -\infty$), set **bl**$[j-1] \leq -$**options.inf_bound**, and to specify a nonexistent upper bound (i.e., $u_j = +\infty$), set **bu**$[j-1] \geq$ **options.inf_bound**, where **options.inf_bound** is one of the optional parameters (default value 10^{20}, see Section 12.2). To specify the jth constraint as an *equality*, set **bl**$[j-1]$ = **bu**$[j-1] = \beta$, say, where $|\beta| <$ **options.inf_bound**. Note that the lower bound corresponding to **iobj** $\neq 0$ must be set to $-\infty$ and stored in **bl**[**n** + |**iobj**| − 1]; similarly, the upper bound must be set to $+\infty$ and stored in **bu**[**n** + |**iobj**| − 1].

On exit: the elements of **bl** and **bu** may have been modified internally, but they are restored on exit.

Constraints:

bl$[j] \leq$ **bu**$[j]$, for $j = 0, 1, \ldots,$ **n** + **m** − 1;
if **bl**$[j]$ = **bu**$[j] = \beta$, $|\beta| <$ **options.inf_bound**;
if **ncnln** $<$ **iobj** $\leq$ **m** or **iobj** $= -1$, **bl**[**n** + |**iobj**| − 1] $\leq -$**options.inf_bound** and
bu[**n** + |**iobj**| − 1] $\geq$ **options.inf_bound**.

15: **xs**[**n** + **m**] – double *Input/Output*

On entry: **xs**[$j-1$], for $j = 1, 2, \ldots,$ **n**, must contain the initial values of the variables, x. In addition, if a 'warm start' is specified by means of the optional parameter **options**.**start** (see Section 12.2) the elements **xs**[**n** + $i-1$], for $i = 1, 2, \ldots,$ **m**, must contain the initial values of the slack variables, s.

On exit: the final values of the variables and slacks (x, s).

16: **ninf** – Integer * *Output*

On exit: the number of constraints that lie outside their bounds by more than the value of the optional parameter **options**.**minor_feas_tol** (default value $= \sqrt{\epsilon}$).

If the *linear* constraints are infeasible, the sum of the infeasibilities of the linear constraints is minimized subject to the upper and lower bounds being satisfied. In this case, **ninf** contains the number of elements of Gx that lie outside their upper or lower bounds. Note that the nonlinear constraints are not evaluated.

Otherwise, the sum of the infeasibilities of the *nonlinear* constraints is minimized subject to the linear constraints and the upper and lower bounds being satisfied. In this case, **ninf** contains the number of elements of $F(x)$ that lie outside their upper or lower bounds.

17: **sinf** – double * *Output*

On exit: the sum of the infeasibilities of constraints that lie outside their bounds by more than the value of the optional parameter **options**.**minor_feas_tol** (default value $= \sqrt{\epsilon}$).

If the *linear* constraints are infeasible, **sinf** contains the sum of the infeasibilities of the linear constraints. Otherwise, **sinf** contains the sum of the infeasibilities of the *nonlinear* constraints.

18: **objf** – double * *Output*

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

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

Note: **comm** is a NAG defined type (see Section 2.3.1.1 in How to Use the NAG Library and its Documentation).

On entry/exit: structure containing pointers for communication to the user-supplied functions **objfun** and **confun**; see the description of **objfun** and **confun** for details. If you do not need to make use of this communication feature the null pointer `NAGCOMM_NULL` may be used in the call to nag_opt_nlp_sparse (e04ugc); **comm** will then be declared internally for use in calls to user-supplied functions.

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

On entry/exit: a pointer to a structure of type Nag_E04_Opt whose members are optional parameters for nag_opt_nlp_sparse (e04ugc). These structure members offer the means of adjusting some of the argument values of the algorithm and on output will supply further details of the results. A description of the members of **options** is given below in Section 12. Some of the results returned in **options** can be used by nag_opt_nlp_sparse (e04ugc) to perform a 'warm start' (see the optional parameter **options**.**start** in Section 12.2).

If any of these optional parameters are required then the structure **options** should be declared and initialized by a call to nag_opt_init (e04xxc) and supplied as an argument to nag_opt_nlp_sparse (e04ugc). However, if the optional parameters are not required the NAG defined null pointer, `E04_DEFAULT`, can be used in the function call.

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

The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).

5.1 Description of Printed Output

Intermediate and final results are printed out by default. The level of printed output can be controlled with the structure members **options.print_level**, **options.minor_print_level**, and **options.print_80ch** (see Section 12.2 and Section 12.3). The default setting of **options.print_level** = Nag_Soln_Iter, **options.print_80ch** = Nag_TRUE, and **options.minor_print_level** = Nag_NoPrint provides a single line of output at each iteration and the final result. This section describes the default printout produced by nag_opt_nlp_sparse (e04ugc).

The following line of summary output (≤ 80 characters) is produced at every major iteration. In all cases, the values of the quantities printed are those in effect *on completion* of the given iteration.

`Maj` is the major iteration count.

`Mnr` is the number of minor iterations required by the feasibility and optimality phases of the QP subproblem. Generally, `Mnr` 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 taken along the computed search direction. On reasonably well-behaved problems, the unit step will be taken as the solution is approached.

`Merit function` is the value of the augmented Lagrangian merit function (6) at the current iterate. This function will decrease at each iteration unless it was necessary to increase the penalty parameters (see Section 11.2). As the solution is approached, `Merit function` will converge to the value of the objective function at the solution.

In elastic mode (see Section 11.2), the merit function is a composite function involving the constraint violations weighted by the value of the optional parameter **options.elastic_wt** (default value $= 1.0$ or 100.0).

If there are no nonlinear constraints present, this entry contains `Objective`, the value of the objective function $f(x)$. In this case, $f(x)$ will decrease monotonically to its optimal value.

`Feasibl` is the value of *rowerr*, the largest element of the scaled nonlinear constraint residual vector defined in the description of the optional parameter **options.major_feas_tol**. The solution is regarded as 'feasible' if `Feasibl` is less than (or equal to) the **options.major_feas_tol** (default value $= \sqrt{\epsilon}$). `Feasibl` will be approximately zero in the neighbourhood of a solution.

If there are no nonlinear constraints present, all iterates are feasible and this entry is not printed.

`Optimal` is the value of *maxgap*, the largest element of the maximum complementarity gap vector defined in the description of the optional parameter **options.major_opt_tol**. The Lagrange multipliers are regarded as 'optimal' if `Optimal` is less than (or equal to) the optional parameter **options.major_opt_tol** (default value $= \sqrt{\epsilon}$). `Optimal` will be approximately zero in the neighbourhood of a solution.

`Cond Hz` is an estimate of the condition number of the reduced Hessian of the Lagrangian (not printed if **ncnln** and **nonln** are both zero). It is the square of the ratio between the largest and smallest diagonal elements of an upper triangular matrix R. This constitutes a lower bound on the condition number of the matrix $R^{\mathrm{T}}R$ that approximates the reduced Hessian. The larger this number, the more difficult the problem.

`PD` is a two-letter indication of the status of the convergence tests involving the feasibility and optimality of the iterates defined in the descriptions of the optional parameters **options.major_feas_tol** and **options.major_opt_tol**. Each letter is `T` if the test is satisfied, and `F` otherwise. The tests indicate whether the values of `Feasibl` and `Optimal` are sufficiently small. For example, `TF` or `TT` is printed if there are no nonlinear constraints present (since all iterates are feasible).

`M` is printed if an extra evaluation of **objfun** and **confun** was needed in order to define an acceptable positive definite quasi-Newton update to the Hessian of the Lagrangian. This modification is only performed when there are nonlinear constraints present.

`m` is printed if, in addition, it was also necessary to modify the update to include an augmented Lagrangian term.

`s` is printed if a self-scaled BFGS (Broyden–Fletcher–Goldfarb–Shanno) update was performed. This update is always used when the Hessian approximation is diagonal, and hence always follows a Hessian reset.

`S` is printed if, in addition, it was also necessary to modify the self-scaled update in order to maintain positive-definiteness.

`n` is printed if no positive definite BFGS update could be found, in which case the approximate Hessian is unchanged from the previous iteration.

`r` is printed if the approximate Hessian was reset after 10 consecutive major iterations in which no BFGS update could be made. The diagonal elements of the approximate Hessian are retained if at least one update has been performed since the last reset. Otherwise, the approximate Hessian is reset to the identity matrix.

`R` is printed if the approximate Hessian has been reset by discarding all but its diagonal elements. This reset will be forced periodically by the values of the optional parameters **options.hess_freq** (default value $= 99999999$) and **options.hess_update** (default value $= 20$). However, it may also be necessary to reset an ill-conditioned Hessian from time to time.

`l` is printed if the change in the variables was limited by the value of the optional parameter **options.major_step_lim** (default value $= 2.0$). If this output occurs frequently during later iterations, it may be worthwhile increasing the value of **options.major_step_lim**.

`c` is printed if central differences have been used to compute the unknown elements 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.

`u` is printed if the QP subproblem was unbounded.

`t` is printed if the minor iterations were terminated because the number of iterations specified by the value of the optional parameter **options.minor_iter_lim** (default value $= 500$) was reached.

`i` is printed if the QP subproblem was infeasible when the function was not in elastic mode. 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 (8) (see Section 11.2). It is also printed if the minimizer of the elastic subproblem does not satisfy the linearized constraints when the function is already in elastic mode. (In this case, a feasible point for the usual QP subproblem may or may not exist.)

`w` is printed if a weak solution of the QP subproblem was found.

The final printout includes a listing of the status of every variable and constraint.

The following describes the printout for each variable.

`Variable` gives the name of the variable. If the optional parameter **options.crnames** $=$ **NULL**, a default name is assigned to the jth variable, for $j = 1, 2, \ldots, n$. Otherwise, the name supplied in **options.crnames**$[j-1]$ is assigned to the jth variable.

`State` gives the state of the variable (`LL` if nonbasic on its lower bound, `UL` if nonbasic on its upper bound, `EQ` if nonbasic and fixed, `FR` if nonbasic and strictly between its bounds, `BS` if basic and `SBS` if superbasic).

A key is sometimes printed before `State` to give some additional information about the state of a variable. Note that unless the optional parameter **options.scale_opt** $= 0$ (default value $= 1$ or 2) 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 current value, there would be no change in the value of the objective function. The values of the basic and superbasic variables *might* change, giving a genuine alternative solution. The values of the Lagrange multipliers *might* also change.

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

`I` *Infeasible*. The variable is basic and is currently violating one of its bounds by more than the value of the optional parameter **options.minor_feas_tol** (default value $= \sqrt{\epsilon}$).

`N` *Not precisely optimal*. The variable is nonbasic. Its reduced gradient is larger than the value of the optional parameter **options.major_feas_tol** (default value $= \sqrt{\epsilon}$).

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

`Lower Bound` is the lower bound specified for the variable. `None` indicates that **bl**$[j-1] \leq -$**options.inf_bound**.

`Upper Bound` is the upper bound specified for the variable. `None` indicates that **bu**$[j-1] \geq$ **options.inf_bound**.

`Lagr Mult` is the Lagrange multiplier for the associated bound. This will be zero if `State` is `FR`. If x is optimal, the multiplier should be non-negative if `State` is `LL`, non-positive if `State` is `UL`, and zero if `State` is `BS` or `SBS`.

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

The meaning of the printout for general constraints is the same as that given above for variables, with 'variable' replaced by 'constraint', n replaced by m, **options.crnames**$[j-1]$) replaced by **options.crnames**$[n+j-1]$, **bl**$[j-1]$ and **bu**$[j-1]$ replaced by **bl**$[n+j-1]$ and **bu**$[n+j-1]$ respectively, and with the following change in the heading:

`Constrnt` gives the name of the general constraint.

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

6 Error Indicators and Warnings

NE_2_INT_ARG_CONS

On entry, **njnln** $= \langle value \rangle$ while **ncnln** $= \langle value \rangle$. These arguments must satisfy **njnln** $= 0$ when **ncnln** $= 0$.

NE_2_INT_OPT_ARG_CONS

On entry, **options.con_check_start** $= \langle value \rangle$ while **options.con_check_stop** $= \langle value \rangle$. These arguments must satisfy **options.con_check_start** $\leq$ **options.con_check_stop**.
(Note that this error may only occur when **options.verify_grad** = Nag_CheckCon or Nag_CheckObjCon.)

On entry, **options.obj_check_start** $= \langle value \rangle$ while **options.obj_check_stop** $= \langle value \rangle$. These arguments must satisfy **options.obj_check_start** $\leq$ **options.obj_check_stop**.

(Note that this error may only occur when **options.verify_grad** = Nag_CheckObj or Nag_CheckObjCon.)

NE_3_INT_ARG_CONS

On entry, **ncnln** = ⟨*value*⟩, **iobj** = ⟨*value*⟩ and **m** = ⟨*value*⟩. These arguments must satisfy **ncnln** < **iobj** ≤ **m** when **iobj** > 0.

NE_ALLOC_FAIL

Dynamic memory allocation failed.

NE_ARRAY_CONS

The contents of array **ka** are not valid.
Constraint: $0 \leq \mathbf{ka}[i+1] - \mathbf{ka}[i] \leq \mathbf{m}$, for $0 \leq i < \mathbf{n}$.

The contents of array **ka** are not valid.
Constraint: $\mathbf{ka}[0] = 0$.

The contents of array **ka** are not valid.
Constraint: $\mathbf{ka}[\mathbf{n}] = \mathbf{nnz}$.

NE_BAD_PARAM

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

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

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

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

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

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

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

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

NE_BASIS_SINGULAR

The basis is singular after 15 attempts to factorize it (and adding slacks when necessary). Either the problem is badly scaled or the value of the optional parameter **options.lu_factor_tol** (default value = 5.0 or 100.0) is too large.

NE_BOUND

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

NE_BOUND_EQ

The lower bound and upper bound for variable ⟨*value*⟩ (array elements **bl**[⟨*value*⟩] and **bu**[⟨*value*⟩]) are equal but they are greater than or equal to **options.inf_bound**.

NE_BOUND_EQ_LCON

The lower bound and upper bound for linear constraint ⟨*value*⟩ (array element **bl**[⟨*value*⟩] and **bu**[⟨*value*⟩]) are equal but they are greater than or equal to **options.inf_bound**.

NE_BOUND_EQ_NLCON

The lower bound and upper bound for nonlinear constraint ⟨*value*⟩ (array element **bl**[⟨*value*⟩] and **bu**[⟨*value*⟩]) are equal but they are greater than or equal to **options.inf_bound**.

NE_BOUND_LCON

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

NE_BOUND_NLCON

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

NE_CANNOT_CALCULATE

The objective and/or constraint functions could not be calculated.

NE_CON_DERIV_ERRORS

Subroutine **confun** appears to be giving incorrect gradients.
The user-provided derivatives of the nonlinear constraint functions computed by **confun** appear to be incorrect. Check that **confun** has been coded correctly and that all relevant elements of the nonlinear constraint Jacobian have been assigned their correct values.

NE_DUPLICATE_ELEMENT

Duplicate sparse matrix element found in row ⟨*value*⟩, column ⟨*value*⟩.

NE_INT_ARG_LT

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

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

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

NE_INT_ARRAY_1

Value ⟨*value*⟩ given to **ka**[⟨*value*⟩] not valid. Correct range for elements of **ka** is ≥ 0.

NE_INT_ARRAY_2

Value ⟨*value*⟩ given to **ha**[⟨*value*⟩] is not valid. Correct range for elements of **ha** is 1 to **m**.

NE_INT_OPT_ARG_GT

On entry, **options.con_check_start** = ⟨*value*⟩.
Constraint: **options.con_check_start** $\leq$ **nonln**.
(Note that this error may only occur when **options.verify_grad** = Nag_CheckCon or Nag_CheckObjCon.)

On entry, **options.con_check_stop** = ⟨*value*⟩.
Constraint: **options.con_check_stop** $\leq$ **nonln**.
(Note that this error may only occur when **options.verify_grad** = Nag_CheckCon or Nag_CheckObjCon.)

On entry, **options.obj_check_start** = ⟨*value*⟩.
Constraint: **options.obj_check_start** $\leq$ **nonln**.
(Note that this error may only occur when **options.verify_grad** = Nag_CheckObj or Nag_CheckObjCon.)

On entry, **options.obj_check_stop** = ⟨*value*⟩.
Constraint: **options.obj_check_stop** $\leq$ **nonln**.
(Note that this error may only occur when **options.verify_grad** = Nag_CheckObj or Nag_CheckObjCon.)

NE_INT_OPT_ARG_LT

On entry, **options.con_check_start** = ⟨*value*⟩.
Constraint: **options.con_check_start** ≥ 1.
(Note that this error may only occur when **options.verify_grad** = Nag_CheckCon or Nag_CheckObjCon.)

On entry, **options.con_check_stop** = ⟨*value*⟩.
Constraint: **options.con_check_stop** ≥ 1.
(Note that this error may only occur when **options.verify_grad** = Nag_CheckCon or Nag_CheckObjCon.)

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

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

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

On entry, **options.obj_check_start** = ⟨*value*⟩.
Constraint: **options.obj_check_start** ≥ 1.
(Note that this error may only occur when **options.verify_grad** = Nag_CheckObj or Nag_CheckObjCon.)

On entry, **options.obj_check_stop** = ⟨*value*⟩.
Constraint: **options.obj_check_stop** ≥ 1.
(Note that this error may only occur when **options.verify_grad** = Nag_CheckObj or Nag_CheckObjCon.)

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.

NE_INVALID_INT_RANGE_1

Value ⟨*value*⟩ given to **ncnln** is not valid. Correct range is 0 to **m**.

Value ⟨*value*⟩ given to **njnln** is not valid. Correct range is (when **ncnln** > 0) 1 to **n**.

Value ⟨*value*⟩ given to **nnz** is not valid. Correct range is 1 to **n** × **m**.

Value ⟨*value*⟩ given to **nonln** is not valid. Correct range is 0 to **n**.

Value ⟨*value*⟩ given to **options.hess_freq** is not valid. Correct range is **options.hess_freq** > 0.

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

Value ⟨*value*⟩ given to **options.iter_lim** is not valid. Correct range is **options.iter_lim** > 0.

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

Value ⟨*value*⟩ given to **options.max_sb** is not valid. Correct range is **options.max_sb** > 0.

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

Value ⟨*value*⟩ given to **options.nsb** is not valid. Correct range is: if **options.start** = Nag_Warm, then **options.nsb** ≥ 0.

Value ⟨*value*⟩ given to **options.part_price** is not valid. Correct range is **options.part_price** > 0.

NE_INVALID_INT_RANGE_2

Value ⟨*value*⟩ given to **options.scale_opt** is not valid. Correct range is 0 ≤ **options.scale_opt** ≤ 2.

NE_INVALID_REAL_RANGE_E

Value ⟨*value*⟩ given to **options.elastic_wt** is not valid. Correct range is **options.elastic_wt** > 0.0.

Value ⟨*value*⟩ given to **options.inf_bound** is not valid. Correct range is **options.inf_bound** > 0.0.

Value ⟨*value*⟩ given to **options.inf_step** is not valid. Correct range is **options.inf_step** > 0.0.

Value ⟨*value*⟩ given to **options.lu_den_tol** is not valid. Correct range is **options.lu_den_tol** ≥ 0.0.

Value ⟨*value*⟩ given to **options.lu_factor_tol** is not valid. Correct range is **options.lu_factor_tol** ≥ 1.0.

Value ⟨*value*⟩ given to **options.lu_sing_tol** is not valid. Correct range is **options.lu_sing_tol** > 0.0.

Value ⟨*value*⟩ given to **options.lu_update_tol** is not valid. Correct range is **options.lu_update_tol** ≥ 1.0.

Value ⟨*value*⟩ given to **options.major_feas_tol** is not valid. Correct range is **options.major_feas_tol** $> \epsilon$.

Value ⟨*value*⟩ given to **options.major_opt_tol** is not valid. Correct range is **options.major_opt_tol** > 0.0.

Value ⟨*value*⟩ given to **options.major_step_lim** is not valid. Correct range is **options.major_step_lim** > 0.0.

Value ⟨*value*⟩ given to **options.minor_feas_tol** is not valid. Correct range is **options.minor_feas_tol** $> \epsilon$.

Value ⟨*value*⟩ given to **options.minor_opt_tol** is not valid. Correct range is **options.minor_opt_tol** > 0.0.

Value ⟨*value*⟩ given to **options.nz_coef** is not valid. Correct range is **options.nz_coef** ≥ 1.0.

Value ⟨*value*⟩ given to **options.pivot_tol** is not valid. Correct range is **options.pivot_tol** > 0.0.

Value ⟨*value*⟩ given to **options.unbounded_obj** is not valid. Correct range is **options.unbounded_obj** > 0.0.

Value ⟨*value*⟩ given to **options.violation_limit** is not valid. Correct range is **options.violation_limit** > 0.0.

NE_INVALID_REAL_RANGE_EE

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

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

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

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

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

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

NE_LIN_NOT_FEASIBLE

No feasible point was found for the linear constraints. Sum of infeasibilities: ⟨*value*⟩.
The problem is infeasible. The linear constraints cannot all be satisfied to within the values of the optional parameter **options.minor_feas_tol** (default value $= \sqrt{\epsilon}$).

NE_MAYBE_UNBOUNDED

Violation limit exceeded. The problem may be unbounded.
Check the values of the optional parameters **options.unbounded_obj** (default value $= 10^{15}$) and **options.inf_step** (default value $= \max\left(bigbnd, 10^{20}\right)$) are not too small. This exit also implies that the objective function is not bounded below (or above in the case of maximization) in the feasible region defined by expanding the bounds by the value of the optional parameter **options.violation_limit** (default value $= 10.0$).

NE_NAME_TOO_LONG

The string pointed to by **options.crnames**[$\langle value \rangle$] is too long. It should be no longer than 8 characters.

NE_NO_IMPROVE

The current point cannot be improved on.
Check that **objfun** and **confun** have been coded correctly and that they are consistent with the values of the optional parameters **options.obj_deriv** and **options.con_deriv** (default value = Nag_TRUE).

NE_NONLIN_NOT_FEASIBLE

No feasible point was found for the nonlinear constraints. Sum of infeasibilities: $\langle value \rangle$.
The problem is infeasible. The nonlinear constraints cannot all be satisfied to within the values of the optional parameter **options.major_feas_tol** (default value $= \sqrt{\epsilon}$).

NE_NOT_APPEND_FILE

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

NE_NOT_CLOSE_FILE

Cannot close file $\langle string \rangle$.

NE_NOT_REQUIRED_ACC

Feasible solution, but required accuracy could not be achieved.
Check that the value of the optional parameter **options.major_opt_tol** (default value $= \sqrt{\epsilon}$) is not too small.

NE_OBJ_BOUND

Invalid lower bound for objective row. Bound should be $\leq -$**options.inf_bound**.

Invalid upper bound for objective row. Bound should be $\geq$ **options.inf_bound**.

NE_OBJ_DERIV_ERRORS

Subroutine **objfun** appears to be giving incorrect gradients.
The user-provided derivatives of the objective function computed by **objfun** appear to be incorrect. Check that **objfun** has been coded correctly and that all relevant elements of the objective gradient have been assigned their correct values.

NE_OPT_NOT_INIT

Options structure not initialized.

NE_OUT_OF_WORKSPACE

There is insufficient workspace for the basis factors, and the maximum allowed number of reallocation attempts, as specified by max_restart, has been reached.

NE_STATE_VAL

options.**state**[⟨*value*⟩] is out of range. **options**.**state**[⟨*value*⟩] = ⟨*value*⟩.

NE_SUPERBASICS_LIMIT

Too many superbasic variables (**options**.**max_sb** = ⟨*value*⟩).
The value of the optional parameter **options**.**max_sb** (default value $= \min(500, \bar{n} + 1, \mathbf{n})$) is too small and should be increased.

NE_TOO_MANY_ITER

Iteration limit (**options**.**iter_lim** = ⟨*value*⟩) exceeded.

NE_TOO_MANY_MAJOR_ITER

Major iteration limit (**options**.**major_iter_lim** = ⟨*value*⟩) exceeded.

NE_TOO_MANY_MINOR_ITER

Minor iteration limit (**options**.**minor_iter_lim** = ⟨*value*⟩) exceeded.

NE_UNBOUNDED

Solution appears to be unbounded.
The problem is unbounded (or badly scaled). The objective function is not bounded below (or above in the case of maximization) in the feasible region because a nonbasic variable can apparently be increased or decreased by an arbitrary amount without causing a basic variable to violate a bound. Add an upper or lower bound to the variable (whose index is printed by default) and rerun nag_opt_nlp_sparse (e04ugc).

NE_USER_STOP

User requested termination, user flag value = ⟨*value*⟩.
This exit occurs if you set **comm**→**flag** to a negative value in **objfun** or **confun**. If **fail** is supplied the value of **fail**.**errnum** will be the same as your setting of **comm**→**flag**.

7 Accuracy

If **options**.**major_feas_tol** is set to 10^{-d} (default value $= \sqrt{\epsilon}$) and **fail**.**code** = NE_NOERROR on exit, then the final value of $f(x)$ should have approximatively d correct digits.

8 Parallelism and Performance

nag_opt_nlp_sparse (e04ugc) is not threaded in any implementation.

9 Further Comments

9.1 Termination Criteria

If nag_opt_nlp_sparse (e04ugc) returns with **fail**.**code** = NE_NOERROR, the iterates have converged to a point x that satisfies the first-order Kuhn–Karesh–Tucker conditions (see Section 11.1) to the accuracy requested by the optional parameters **options**.**major_feas_tol** (default value $= \sqrt{\epsilon}$) and **options**.**major_opt_tol** (default value $= \sqrt{\epsilon}$).

10 Example

This example is a reformulation of Problem 74 from Hock and Schittkowski (1981) and involves minimization of the nonlinear function

$$f(x) = 10^{-6}x_3^3 + \frac{2}{3} \times 10^{-6}x_4^3 + 3x_3 + 2x_4$$

subject to the bounds

$$\begin{aligned} -0.55 \leq x_1 \leq 0.55 \\ -0.55 \leq x_2 \leq 0.55 \\ 5 \leq x_3 \leq 1200 \\ 5 \leq x_4 \leq 1200 \end{aligned}$$

to the nonlinear constraints

$$\begin{aligned} 1000\sin(-x_1 - 0.25) + 1000\sin(-x_2 - 0.25) \quad - x_3 &= -894.8 \\ 1000\sin(x_1 - 0.25) \quad + 1000\sin(x_1 - x_2 - 0.25) - x_4 &= -894.8 \\ 1000\sin(x_2 - 0.25) \quad + 1000\sin(x_2 - x_1 - 0.25) &= -1294.8 \end{aligned}$$

and to the linear constraints

$$\begin{aligned} -x_1 + x_2 \geq -0.55 \\ x_1 - x_2 \geq -0.55 \end{aligned}$$

The initial point, which is infeasible, is

$$x_0 = (0, 0, 0, 0)^{\mathrm{T}},$$

and $f(x_0) = 0$.

The optimal solution (to five figures) is

$$x^* = (0.11887, -0.39623, 679.94, 1026.0)^{\mathrm{T}},$$

and $f(x^*) = 5126.4$. All the nonlinear constraints are active at the solution.

The use of the interface to nag_opt_nlp_sparse (e04ugc) for this particular example is briefly illustrated below. First, note that because of the constraints on the definitions of nonlinear Jacobian variables and nonlinear objective variables in the interface to nag_opt_nlp_sparse (e04ugc), the first objective variables x_1 and x_2 are considered as nonlinear objective variables. Thus, **nonln** $= 4$, and there are **njnln** $= 2$ nonlinear Jacobian variables (x_1 and x_2). (The alternative would have consisted in reordering the problem to have **nonln** $= 2$ nonlinear objective variables and **njnln** $= 4$ nonlinear constraint variables, but, as mentioned earlier, it is preferable to keep the size of the nonlinear Jacobian (J) small, having **nonln** $>$ **njnln**.)

The Jacobian matrix A is the **m** $= 6$ by **n** $= 4$ matrix below

$$A = \begin{pmatrix} \mathbf{conjac}[0] & \mathbf{conjac}[3] & -1 & 0 \\ \mathbf{conjac}[1] & \mathbf{conjac}[4] & 0 & -1 \\ \mathbf{conjac}[2] & \mathbf{conjac}[5] & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 3 & 2 \end{pmatrix},$$

where zeros are not stored, each column represents a variable, each row a constraint (except the free row), and the **conjac**$[i]$ entries reflect the structure of the Jacobian J corresponding to the nonlinear constraints. The first 3 rows correspond to the **ncnln** $= 3$ nonlinear constraints, rows 4 and 5 define the 2 linear constraints and there is finally an **iobj** $= 6$th free row defining the linear part of the objective function, $3x_3 + 2x_4$.

A contains **nnz** $= 14$ nonzero elements of which six entries define the structure of J. In this case all entries in J are defined in the supplied function **confun** and there is no constant value that we want to pass only once via A, so all entries in the corresponding array **a** corresponding to J can just be initialized to dummy values (here $1.0\mathrm{e}+25$). Effective Jacobian values will be provided in the argument **conjac**$[i-1]$, for $i = 1, 2, \ldots,$ **nnzjac**, **nnzjac** $= 6$, in the function **confun**. Note also that in this simple example, J is indeed full; otherwise, the structure of A should reflect the sparsity of J.

This example includes source code to store the matrix A in the arrays **a**, **ha**, **ka**, based on the simple format from the data file.

Finally, the lower and upper bounds are defined by $\mathbf{bl} = (-0.55, -0.55, 0.0, 0.0, -894.6, -894.6, -1294.8, -0.55, -0.55, -1.0\text{e}+25)^{\mathrm{T}}$, and $\mathbf{bu} = (0.55, 0.55, 1200.0, 1200.0, -894.6, -894.6, -1294.8, 1.0\text{e}+25, 1.0\text{e}+25, 1.0\text{e}+25)^{\mathrm{T}}$.

The first $\mathbf{n} = 4$ elements of **bl** and **bu** are simple bounds on the variables; the next 3 elements are bounds on the nonlinear constraints; the next 2 elements are bounds on the linear constraints; and finally, the last (unbounded) element corresponds to the free row.

The **options** structure is declared and initialized by nag_opt_init (e04xxc). The **options**.**crnames** member is assigned to the array of character strings into which the column and row names were read and the **options**.**major_iter** member is assigned a value of 100. Two options are read from the data file by use of nag_opt_read (e04xyc). Note that, unlike for some other optimization functions, optional parameters to nag_opt_nlp_sparse (e04ugc) are not checked inside nag_opt_read (e04xyc); they are checked inside the main call to nag_opt_nlp_sparse (e04ugc).

On return from nag_opt_nlp_sparse (e04ugc), the solution is perturbed slightly and some further options set, selecting a warm start and a reduced level of printout. nag_opt_nlp_sparse (e04ugc) is then called for a second time. Finally, the memory freeing function nag_opt_free (e04xzc) is used to free the memory assigned by nag_opt_nlp_sparse (e04ugc) to the pointers in the options structure. You must **not** use the standard C function `free()` for this purpose.

10.1 Program Text

```
/* nag_opt_nlp_sparse (e04ugc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * NAG C Library
 *
 * Mark 26, 2016.
 *
 */

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

#ifdef __cplusplus
extern "C"
{
#endif
  static void NAG_CALL confun(Integer ncnln, Integer njnln,
                              Integer nnzjac, const double x[], double conf[],
                              double conjac[], Nag_Comm *comm);

  static void NAG_CALL objfun(Integer nonln,
                              const double x[], double *objf,
                              double objgrad[], Nag_Comm *comm);
#ifdef __cplusplus
}
#endif

#define NAMES(I, J) names[(I)*9+J]

int main(void)
{
  const char *optionsfile = "e04ugce.opt";
  Integer exit_status = 0, *ha = 0, i, icol, iobj, j, jcol, *ka = 0, m, n,
          ncnln;
  Integer ninf, njnln, nnz, nonln;
  Nag_E04_Opt options;
  char **crnames = 0, *names = 0;
```

```
  double *a = 0, *bl = 0, *bu = 0, obj, sinf, *xs = 0;
  Integer verbose_output;
  Nag_Comm comm;
  NagError fail;

  INIT_FAIL(fail);

  printf("nag_opt_nlp_sparse (e04ugc) Example Program Results\n");
  fflush(stdout);

  /* Skip heading in data file */
#ifdef _WIN32
  scanf_s(" %*[^\n]");
#else
  scanf(" %*[^\n]");
#endif
  /* Read the problem dimensions */
#ifdef _WIN32
  scanf_s(" %*[^\n]");
#else
  scanf(" %*[^\n]");
#endif
#ifdef _WIN32
  scanf_s("%" NAG_IFMT "%" NAG_IFMT "", &n, &m);
#else
  scanf("%" NAG_IFMT "%" NAG_IFMT "", &n, &m);
#endif
  /* Read NCNLN, NONLN and NJNLN from data file. */
#ifdef _WIN32
  scanf_s(" %*[^\n]");
#else
  scanf(" %*[^\n]");
#endif
#ifdef _WIN32
  scanf_s("%" NAG_IFMT "%" NAG_IFMT "%" NAG_IFMT "", &ncnln, &nonln, &njnln);
#else
  scanf("%" NAG_IFMT "%" NAG_IFMT "%" NAG_IFMT "", &ncnln, &nonln, &njnln);
#endif
  /* Read NNZ, IOBJ */
#ifdef _WIN32
  scanf_s(" %*[^\n]");
#else
  scanf(" %*[^\n]");
#endif
#ifdef _WIN32
  scanf_s("%" NAG_IFMT "%" NAG_IFMT "", &nnz, &iobj);
#else
  scanf("%" NAG_IFMT "%" NAG_IFMT "", &nnz, &iobj);
#endif

  if (!(a = NAG_ALLOC(nnz, double)) ||
      !(bl = NAG_ALLOC(n + m, double)) ||
      !(bu = NAG_ALLOC(n + m, double)) ||
      !(xs = NAG_ALLOC(n + m, double)) ||
      !(ha = NAG_ALLOC(nnz, Integer)) ||
      !(ka = NAG_ALLOC(n + 1, Integer)) ||
      !(crnames = NAG_ALLOC(n + m, char *)) ||
      !(names = NAG_ALLOC((n + m) * 9, char))
         )
  {
    printf("Allocation failure\n");
    exit_status = 1;
    goto END;
  }

  /* Read the column and row names */
#ifdef _WIN32
  scanf_s(" %*[^\n]");
#else
  scanf(" %*[^\n]");
#endif
```

```
#ifdef _WIN32
  scanf_s(" %*[^']");
#else
  scanf(" %*[^']");
#endif
  for (i = 0; i < n + m; ++i) {
#ifdef _WIN32
    scanf_s(" '%8c'", &NAMES(i, 0), 9);
#else
    scanf(" '%8c'", &NAMES(i, 0));
#endif
    NAMES(i, 8) = '\setminus 0';
    crnames[i] = &NAMES(i, 0);
  }

  /* read the matrix and set up ka. */
  jcol = 1;
  ka[jcol - 1] = 0;
#ifdef _WIN32
  scanf_s(" %*[^\n]");
#else
  scanf(" %*[^\n]");
#endif
  for (i = 0; i < nnz; ++i) {
    /* a[i] stores (ha[i], icol) element of matrix */
#ifdef _WIN32
    scanf_s("%lf%" NAG_IFMT "%" NAG_IFMT "", &a[i], &ha[i], &icol);
#else
    scanf("%lf%" NAG_IFMT "%" NAG_IFMT "", &a[i], &ha[i], &icol);
#endif
    if (icol < jcol) {
      /* Elements not ordered by increasing column index. */
      printf("Element in column%5" NAG_IFMT " found after element in"
             " column%5" NAG_IFMT ". Problem abandoned.\n", icol, jcol);
      exit_status = 1;
      goto END;
    }
    else if (icol == jcol + 1) {
      /* Index in a of the start of the icol-th column equals i. */
      ka[icol - 1] = i;
      jcol = icol;
    }
    else if (icol > jcol + 1) {
      /* Index in a of the start of the icol-th column equals i,
       *  but columns jcol+1,jcol+2,...,icol-1 are empty. Set the
       *  corresponding elements of ka to i.
       */
      for (j = jcol + 1; j <= icol - 1; ++j)
        ka[j - 1] = i;

      ka[icol - 1] = i;
      jcol = icol;
    }
  }
  ka[n] = nnz;
  if (n > icol) {
    /* Columns N,N-1,...,ICOL+1 are empty. Set the
     *  corresponding elements of ka accordingly. */
    for (j = icol; j <= n - 1; ++j)
      ka[j] = nnz;
  }

  /* Read the bounds */
#ifdef _WIN32
  scanf_s(" %*[^\n]");
#else
  scanf(" %*[^\n]");
#endif
  for (i = 0; i < n + m; ++i)
#ifdef _WIN32
    scanf_s("%lf", &bl[i]);
```

```
#else
    scanf("%lf", &bl[i]);
#endif
#ifdef _WIN32
  scanf_s(" %*[^\n]");
#else
  scanf(" %*[^\n]");
#endif
  for (i = 0; i < n + m; ++i)
#ifdef _WIN32
    scanf_s("%lf", &bu[i]);
#else
    scanf("%lf", &bu[i]);
#endif

  /* Read the initial estimate of x */
#ifdef _WIN32
  scanf_s(" %*[^\n]");
#else
  scanf(" %*[^\n]");
#endif
  for (i = 0; i < n; ++i)
#ifdef _WIN32
    scanf_s("%lf", &xs[i]);
#else
    scanf("%lf", &xs[i]);
#endif

  /* Initialize the options structure */
  /* nag_opt_init (e04xxc).
   * Initialization function for option setting
   */
  nag_opt_init(&options);

  /* Set this to 1 to cause e04ugc to produce intermediate
     progress output */
  verbose_output = 0;

  /* Read some option values from standard input */
  /* nag_opt_read (e04xyc).
   * Read options from a text file
   */
  nag_opt_read("e04ugc", optionsfile, &options,
               (Nag_Boolean)(verbose_output==1), "stdout", &fail);
  /* Set some other options directly */
  options.major_iter_lim = 100;
  options.crnames = crnames;

  if (verbose_output == 0)
    {
      options.list = Nag_FALSE;
      options.print_level = Nag_NoPrint;
      options.print_deriv = Nag_D_NoPrint;
    }

  /* Solve the problem. */
  /* nag_opt_nlp_sparse (e04ugc), see above. */
  nag_opt_nlp_sparse(confun, objfun, n, m,
                     ncnln, nonln, njnln, iobj, nnz,
                     a, ha, ka, bl, bu, xs,
                     &ninf, &sinf, &obj, &comm, &options, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_opt_nlp_sparse (e04ugc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }

  if (verbose_output == 0)
    {
      printf("\n");
      printf("Final objective value = %12.3f\n", obj);
```

```
      printf("Optimal X = ");
      for (i = 1; i <= n; ++i) {
        printf("%9.3f%s", xs[i - 1], i % 7 == 0 || i == n ? "\n" : " ");
      }
    }

  /* We perturb the solution and solve the
   * same problem again using a warm start.
   */
  printf("\nA run of the same example with a warm start:\n");
  printf("-------------------------------------------\n");
  options.start = Nag_Warm;

  /* Modify some printing options */
  options.print_deriv = Nag_D_NoPrint;
  if (verbose_output == 1)
    options.print_level = Nag_Iter;
  else
    options.print_level = Nag_NoPrint;

  /* Perturb xs */
  for (i = 0; i < n + m; i++)
    xs[i] += 0.2;

  /* Reset multiplier estimates to 0.0 */
  if (ncnln > 0) {
    for (i = 0; i < ncnln; i++)
      options.lambda[n + i] = 0.0;
  }
  /* Solve the problem again. */
  /* nag_opt_nlp_sparse (e04ugc), see above. */
  fflush(stdout);
  nag_opt_nlp_sparse(confun, objfun, n, m,
                     ncnln, nonln, njnln, iobj, nnz,
                     a, ha, ka, bl, bu, xs,
                     &ninf, &sinf, &obj, &comm, &options, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_opt_nlp_sparse (e04ugc).\n%s\n", fail.message);
    exit_status = 1;
  }

  if (verbose_output == 0)
    {
      printf("Final objective value = %12.3f\n", obj);
      printf("Optimal X = ");
      for (i = 1; i <= n; ++i) {
        printf("%9.3f%s", xs[i - 1], i % 7 == 0 || i == n ? "\n" : " ");
      }
    }

  /* Free memory allocated by nag_opt_nlp_sparse (e04ugc) to pointers in options
   */
  /* nag_opt_free (e04xzc).
   * Memory freeing function for use with option setting
   */
  nag_opt_free(&options, "all", &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_opt_free (e04xzc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }

END:
  NAG_FREE(a);
  NAG_FREE(bl);
  NAG_FREE(bu);
  NAG_FREE(xs);
  NAG_FREE(ha);
  NAG_FREE(ka);
  NAG_FREE(crnames);
  NAG_FREE(names);
```

```
  return exit_status;
}

/* Subroutine */
static void NAG_CALL confun(Integer ncnln, Integer njnln, Integer nnzjac,
                            const double x[], double conf[], double conjac[],
                            Nag_Comm *comm)
{
#define CONJAC(I) conjac[(I) -1]
#define CONF(I)   conf[(I) -1]
#define X(I)      x[(I) -1]
  /* Compute the nonlinear constraint functions and their Jacobian. */
  if (comm->flag == 0 || comm->flag == 2) {
    CONF(1) = sin(-X(1) - 0.25) * 1e3 + sin(-X(2) - 0.25) * 1e3;
    CONF(2) = sin(X(1) - 0.25) * 1e3 + sin(X(1) - X(2) - 0.25) * 1e3;
    CONF(3) = sin(X(2) - X(1) - 0.25) * 1e3 + sin(X(2) - 0.25) * 1e3;
  }
  if (comm->flag == 1 || comm->flag == 2) {
    /* Nonlinear Jacobian elements for column 1.0 */
    CONJAC(1) = cos(-X(1) - 0.25) * -1e3;
    CONJAC(2) = cos(X(1) - 0.25) * 1e3 + cos(X(1) - X(2) - 0.25) * 1e3;
    CONJAC(3) = cos(X(2) - X(1) - 0.25) * -1e3;
    /* Nonlinear Jacobian elements for column 2.0 */
    CONJAC(4) = cos(-X(2) - 0.25) * -1e3;
    CONJAC(5) = cos(X(1) - X(2) - 0.25) * -1e3;
    CONJAC(6) = cos(X(2) - X(1) - 0.25) * 1e3 + cos(X(2) - 0.25) * 1e3;
  }
}

static void NAG_CALL objfun(Integer nonln, const double x[], double *objf,
                            double objgrad[], Nag_Comm *comm)
{
#define OBJGRAD(I) objgrad[(I) -1]
#define X(I)       x[(I) -1]
  /* Compute the nonlinear part of the objective function and its grad */
  if (comm->flag == 0 || comm->flag == 2)
    *objf = X(3) * X(3) * X(3) * 1e-6 + X(4) * X(4) * X(4) * 2e-6 / 3.0;
  if (comm->flag == 1 || comm->flag == 2) {
    OBJGRAD(1) = 0.0;
    OBJGRAD(2) = 0.0;
    OBJGRAD(3) = X(3) * X(3) * 3e-6;
    OBJGRAD(4) = X(4) * X(4) * 2e-6;
  }
}
```

10.2 Program Data

```
nag_opt_nlp_sparse (e04ugc) Example Program Data

Values of n and m
4  6

Values of ncnln, nonln and njnln
3  4  2

Values of nnz and iobj
14  6

Columns and rows names
'Varble 1'  'Varble 2'  'Varble 3'  'Varble 4'  'NlnCon 1'
'NlnCon 2'  'NlnCon 3'  'LinCon 1'  'LinCon 2'  'Free Row'

Matrix nonzeros: value, row index, column index
 1.0E+25   1   1
 1.0E+25   2   1
 1.0E+25   3   1
     1.0   5   1
    -1.0   4   1
 1.0E+25   1   2
```

```
 1.0E+25   2   2
 1.0E+25   3   2
     1.0   5   2
    -1.0   4   2
     3.0   6   3
    -1.0   1   3
    -1.0   2   4
     2.0   6   4

Lower bounds
-0.55     -0.55      0.0       0.0     -894.8   -894.8   -1294.8  -0.55
-0.55     -1.0E+25

Upper bounds
 0.55      0.55      1200.0    1200.0  -894.8   -894.8   -1294.8   1.0E+25
 1.0E+25   1.0E+25

Initial estimate of X
 0.0  0.0  0.0  0.0
nag_opt_nlp_sparse (e04ugc) Example Program Optional Parameters

Begin e04ugc
minor_iter_lim = 20
iter_lim = 30
End
```

10.3 Program Results

```
nag_opt_nlp_sparse (e04ugc) Example Program Results

Final objective value =     5126.498
Optimal X =     0.119    -0.396   679.945  1026.067

A run of the same example with a warm start:
-------------------------------------------
Final objective value =     5126.498
Optimal X =     0.119    -0.396   679.945  1026.067
```

11 Further Description

nag_opt_nlp_sparse (e04ugc) implements a sequential quadratic programming (SQP) method that obtains search directions from a sequence of quadratic programming (QP) subproblems. This section gives a detailed description of the algorithms used by nag_opt_nlp_sparse (e04ugc). This, and possibly the next section, Section 12, may be omitted if the more sophisticated features of the algorithm and software are not currently of interest.

11.1 Overview

Here we briefly summarise the main features of the method and introduce some terminology. Where possible, explicit reference is made to the names of variables that are arguments of the function or appear in the printed output. Further details can be found in Gill *et al.* (2002).

At a solution of (1), some of the constraints will be *active*, i.e., satisfied exactly. Let

$$r(x) = \begin{pmatrix} x \\ F(x) \\ Gx \end{pmatrix},$$

and $\mathcal{G}$ denote the set of indices of $r(x)$ corresponding to active constraints at an arbitrary point x. Let $r_j'(x)$ denote the usual *derivative* of $r_j(x)$, which is the row vector of first partial derivatives of $r_j(x)$ (see Ortega and Rheinboldt (1970)). The vector $r_j'(x)$ comprises the jth row of $r'(x)$ so that

$$r'(x) = \begin{pmatrix} I \\ J(x) \\ G \end{pmatrix},$$

where $J(x)$ is the Jacobian of $F(x)$.

A point x is a *first-order Kuhn–Karesh–Tucker (KKT) point* for (1) (see, e.g., Powell (1974)) if the following conditions hold:

(a) x is feasible;

(b) there exists a vector λ (*the Lagrange multiplier vector for the bound and general constraints*) such that

$$g(x) = r'(x)^{\mathrm{T}}\lambda = \begin{pmatrix} I & J(x)^{\mathrm{T}} & G^{\mathrm{T}} \end{pmatrix}\lambda, \tag{4}$$

where g is the gradient of f evaluated at x;

(c) the Lagrange multiplier λ_j associated with the jth constraint satisfies $\lambda_j = 0$ if $l_j < r_j(x) < u_j$; $\lambda_j \geq 0$ if $l_j = r_j(x)$; $\lambda_j \leq 0$ if $r_j(x) = u_j$; and λ_j can have any value if $l_j = u_j$.

An equivalent statement of the condition (4) is

$$Z^{\mathrm{T}}g(x) = 0,$$

where Z is a matrix defined as follows. Consider the set N of vectors orthogonal to the gradients of the active constraints, i.e.,

$$N = \Big\{ z \quad | \quad r_j'(x)z = 0 \quad \text{for all} \quad j \in \mathcal{G} \Big\}.$$

The columns of Z may then be taken as any basis for the vector space N. The vector $Z^{\mathrm{T}}g$ is termed the *reduced gradient* of f at x. Certain additional conditions must be satisfied in order for a first-order KKT point to be a solution of (1) (see, e.g., Powell (1974)).

The basic structure of nag_opt_nlp_sparse (e04ugc) 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 x^* that satisfies the first-order KKT optimality conditions. At each iterate 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 $Gx - s_L = 0$ and the nonlinear constraint linearization

$$F(x_k) + F'(x_k)(x - x_k) - s_N = 0,$$

where $F'(x_k)$ denotes the *Jacobian matrix*, whose rows are the first partial derivatives of $F(x)$ evaluated at the point x_k. The QP constraints therefore comprise the m linear constraints

$$\begin{array}{llll} F'(x_k)x & -s_N & & = -F(x_k) + F'(x_k)x_k, \\ Gx & & -s_L & = 0, \end{array}$$

where x and $s = (s_N, s_L)^{\mathrm{T}}$ are bounded above and below by u and l as before. If the m by n matrix A and m element vector b are defined as

$$A = \begin{pmatrix} F'(x_k) \\ G \end{pmatrix} \quad \text{and} \quad b = \begin{pmatrix} -F(x_k) + F'(x_k)x_k \\ 0 \end{pmatrix},$$

then the QP subproblem can be written as

$$\underset{x,s}{\text{minimize}} q(x) \quad \text{subject to} \quad Ax - s = b, \quad l \leq \begin{Bmatrix} x \\ s \end{Bmatrix} \leq u, \tag{5}$$

where $q(x)$ is a quadratic approximation to a modified Lagrangian function (see Gill *et al.* (2002)).

The linear constraint matrix A is stored in the arrays **a**, **ha** and **ka** (see Section 5). This allows you to specify the sparsity pattern of nonzero elements in $F'(x)$ and G, and identify any nonzero elements that remain constant throughout the minimization.

Solving the QP subproblem is itself an iterative procedure, with the *minor* iterations of an SQP method being the iterations of the QP method. At each minor iteration, the constraints $Ax - s = b$ are (conceptually) partitioned into the form

$$Bx_B + Sx_S + Nx_N = b,$$

where the *basis matrix* B is square and nonsingular. The elements of x_B, x_S and x_N are called the *basic*, *superbasic* and *nonbasic* variables respectively; they are a permutation of the elements of x and s. At a QP solution, the basic and superbasic variables will lie somewhere between their bounds, while the nonbasic variables will be equal to one of their upper or lower bounds. At each minor 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 function $q(x)$ or sum of infeasibilities (as appropriate). 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 if there are no nonlinear constraints in (1) and $f(x)$ is linear.

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 decreased by one.

Associated with each of the m equality constraints $Ax - s = b$ is a *dual variable* π_i. Similarly, each variable in (x, s) has an associated *reduced gradient* d_j (also known as a *reduced cost*). The reduced gradients for the variables x are the quantities $g - A^{\mathrm{T}}\pi$, where g is the gradient of the QP objective function $q(x)$; and the reduced gradients for the slack variables s are the dual variables π. The QP subproblem (5) 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 is found by slightly relaxing these conditions on d_j (see the description of the optional parameter **options.minor_opt_tol**).

After a QP subproblem has been solved, new estimates of the solution to (1) are computed using a linesearch on the augmented Lagrangian merit function

$$\mathcal{M}(x, s, \pi) = f(x) - \pi^{\mathrm{T}}(F(x) - s_N) + \frac{1}{2}(F(x) - s_N)^{\mathrm{T}} D (F(x) - s_N), \tag{6}$$

where D is a diagonal matrix of penalty parameters. If (x_k, s_k, π_k) denotes the current estimate of the solution and $(\hat{x}, \hat{s}, \hat{\pi})$ denotes the optimal QP solution, the linesearch determines a step α_k (where $0 < \alpha_k \leq 1$) such that the new point

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

produces a *sufficient decrease* in the merit function (6). When necessary, the penalties in D are increased by the minimum-norm perturbation that ensures descent for $\mathcal{M}$ (see Gill *et al.* (1992)). As in nag_opt_nlp (e04ucc), s_N is adjusted to minimize the merit function as a function of s prior to the solution of the QP subproblem. Further details can be found in Eldersveld (1991) and Gill *et al.* (1986).

11.2 Treatment of Constraint Infeasibilities

nag_opt_nlp_sparse (e04ugc) makes explicit allowance for infeasible constraints. Infeasible linear constraints are detected first by solving a problem of the form

$$\underset{x,v,w}{\text{minimize}} e^{\mathrm{T}}(v + w) \quad \text{subject to} \quad l \leq \begin{Bmatrix} x \\ Gx - u + w \end{Bmatrix} \leq u, \quad v \geq 0, \quad w \geq 0, \tag{7}$$

where $e = (1, 1, \ldots, 1)^{\mathrm{T}}$. This is equivalent to minimizing the sum of the general linear constraint violations subject to the simple bounds. (In the linear programming literature, the approach is often called *elastic programming*.)

If the linear constraints are infeasible (i.e., $v \neq 0$ or $w \neq 0$), the function terminates without computing the nonlinear functions.

If the linear constraints are feasible, all subsequent iterates will satisfy the linear constraints. (Such a strategy allows linear constraints to be used to define a region in which $f(x)$ and $F(x)$ can be safely evaluated.) The function proceeds to solve (1) as given, using search directions obtained from a sequence of QP subproblems (5). Each QP subproblem minimizes a quadratic model of a certain Lagrangian function subject to linearized constraints. An augmented Lagrangian merit function (6) is reduced along each search direction to ensure convergence from any starting point.

The function enters 'elastic' mode if the QP subproblem proves to be infeasible or unbounded (or if the dual variables π for the nonlinear constraints become 'large') by solving a problem of the form

$$\underset{x,v,w}{\text{minimize}} \bar{f}(x,v,w) \quad \text{subject to} \quad l \leq \begin{Bmatrix} x \\ F(x) - v + w \\ Gx \end{Bmatrix} \leq u, \quad v \geq 0, \quad w \geq 0, \tag{8}$$

where

$$\bar{f}(x,v,w) = f(x) + \gamma e^{\mathrm{T}}(v+w) \tag{9}$$

is called a *composite objective* and γ is a non-negative argument (the *elastic weight*). If γ is sufficiently large, this is equivalent to minimizing the sum of the nonlinear constraint violations subject to the linear constraints and bounds. A similar l_1 formulation of (1) is fundamental to the Sl_1QP algorithm of Fletcher (1984). See also Conn (1973).

12 Optional Parameters

A number of optional input and output arguments to nag_opt_nlp_sparse (e04ugc) are available through the structure argument **options**, type Nag_E04_Opt. An argument may be selected by assigning an appropriate value to the relevant structure member; those arguments not selected will be assigned default values. If no use is to be made of any of the optional parameters you should use the NAG defined null pointer, `E04_DEFAULT`, in place of **options** when calling nag_opt_nlp_sparse (e04ugc); the default settings will then be used for all arguments.

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

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

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

12.1 Optional Parameter Checklist and Default Values

For easy reference, the following list shows the members of **options** which are valid for nag_opt_nlp_sparse (e04ugc) together with their default values where relevant. The number ϵ is a generic notation for ***machine precision*** (see nag_machine_precision (X02AJC)).

`Nag_Start start`	Nag_Cold
`Boolean list`	Nag_TRUE
`Boolean print_80ch`	Nag_TRUE
`Nag_PrintType print_level`	Nag_Soln_Iter
`Nag_PrintType minor_print_level`	Nag_NoPrint
`Nag_DPrintType print_deriv`	Nag_D_Print
`char outfile[80]`	`stdout`
`char **crnames`	**NULL**

`Boolean obj_deriv`	Nag_TRUE
`Boolean con_deriv`	Nag_TRUE
`Nag_GradChk verify_grad`	Nag_SimpleCheck
`Integer obj_check_start`	1
`Integer obj_check_stop`	**nonln**
`Integer con_check_start`	1
`Integer con_check_stop`	**njnln**
`double f_diff_int`	$\sqrt{\textbf{options.f\_prec}}$
`double c_diff_int`	$\textbf{options.f\_prec}^{0.33}$
`Nag_CrashType crash`	Nag_NoCrash or Nag_CrashThreeTimes
`Integer expand_freq`	10000
`Integer factor_freq`	50 or 100
`Integer fcheck`	60
`Integer hess_freq`	99999999
`Integer hess_update`	20
`Integer iter_lim`	10000
`Integer major_iter_lim`	1000
`Integer minor_iter_lim`	500
`Integer part_price`	1 or 10
`Integer scale_opt`	1 or 2
`Integer max_sb`	$\min(500, \mathbf{n}, \bar{n}+1)$
`double crash_tol`	0.1
`double elastic_wt`	1.0 or 100.0
`double f_prec`	$\epsilon^{0.8}$
`double inf_bound`	10^{20}
`double linesearch_tol`	0.9
`double lu_den_tol`	0.6
`double lu_sing_tol`	$\epsilon^{0.67}$
`double lu_factor_tol`	5.0 or 100.0
`double lu_update_tol`	5.0 or 10.0
`double major_feas_tol`	$\sqrt{\epsilon}$
`double major_opt_tol`	$\sqrt{\epsilon}$
`double major_step_lim`	2.0
`double minor_feas_tol`	$\sqrt{\epsilon}$
`double minor_opt_tol`	$\sqrt{\epsilon}$
`double nz_coef`	5.0
`double pivot_tol`	$\epsilon^{0.67}$
`double scale_tol`	0.9
`double unbounded_obj`	10^{15}

`double inf_step`	$\max\left(\textbf{options.inf\_bound}, 10^{20}\right)$
`double violation_limit`	10.0
`Boolean deriv_linesearch`	Nag_TRUE
`Boolean feas_exit`	Nag_FALSE
`Nag_HessianType hess_storage`	Nag_HessianFull or Nag_HessianLimited
`Nag_DirectionType direction`	Nag_Minimize
`Integer *state`	size $\mathbf{n} + \mathbf{m}$
`double *lambda`	size $\mathbf{n} + \mathbf{m}$
`Integer iter`	
`Integer major_iter`	
`Integer nsb`	
`Integer nf`	

12.2 Description of the Optional Parameters

start – Nag_Start Default = Nag_Cold

On entry: indicates how a starting basis is to be obtained.

If **options.start** = Nag_Cold, then an initial Crash procedure will be used to choose an initial basis.

If **options.start** = Nag_Warm, then you must provide a valid definition of the optional parameters **options.state** and **options.nsb**. (These may be the output of a previous call.)

A warm start will be advantageous if a good estimate of the initial working set is available – for example, when nag_opt_nlp_sparse (e04ugc) is called repeatedly to solve related problems.

Constraint: **options.start** = Nag_Cold or Nag_Warm.

list – Nag_Boolean Default = Nag_TRUE

On entry: if **options.list** = Nag_TRUE the argument settings in the call to nag_opt_nlp_sparse (e04ugc) will be printed. The actual options printed can vary depending on the problem type being solved.

print_80ch – Nag_Boolean Default = Nag_TRUE

On entry: controls the maximum length of each line of output produced by major and minor iterations and by the printing of the solution.

If **options.print_80ch** = Nag_TRUE (the default), then a maximum of 80 characters per line is printed.

If **options.print_80ch** = Nag_FALSE, then a maximum of 120 characters per line is printed.

(See also **options.print_level** and **options.minor_print_level** below.)

print_level – Nag_PrintType Default = Nag_Soln_Iter

On entry: the level of results printout produced by nag_opt_nlp_sparse (e04ugc) at each major iteration, as indicated below. A detailed description of the printed output is given in Section 5.1 and Section 12.3. (See also **options.minor_print_level**, below.)

Nag_NoPrint	No output.
Nag_Soln	The final solution only.
Nag_Iter	One line of output for each major iteration (no printout of the final solution).
Nag_Soln_Iter	The final solution and one line of output for each iteration.
Nag_Soln_Iter_Full	The final solution, one line of output for each major iteration, matrix statistics (initial status of rows and columns, number of elements, density, biggest and

smallest elements, etc.), details of the scale factors resulting from the scaling procedure (if **options**.**scale_opt** = 1 or 2; see below), basis factorization statistics and details of the initial basis resulting from the Crash procedure (if **options**.**start** = Nag_Cold and **options**.**crash** ≠ Nag_NoCrash).

Note that the output for each line of major iteration and for the solution printout contains a maximum of 80 characters if **options**.**print_80ch** = Nag_TRUE, and a maximum of 120 characters otherwise. However, if **options**.**print_level** = Nag_Soln_Iter_Full, some printout may exceed 80 characters even when **options**.**print_80ch** = Nag_TRUE.

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

minor_print_level – Nag_PrintType Default = Nag_NoPrint

On entry: controls the amount of printout produced by the minor iterations of nag_opt_nlp_sparse (e04ugc) (i.e., the iterations of the quadratic programming algorithm), as indicated below. A detailed description of the printed output is given in Section 9.1 (default output at each iteration) and in Section 12.3. (See also **options**.**print_level**.)

If **options**.**minor_print_level** = Nag_NoPrint, no output is produced.

If **options**.**minor_print_level** = Nag_Iter, the following output is produced for each minor iteration:

if **options**.**print_80ch** = Nag_TRUE, one line of summary output (≤ 80 characters);

if **options**.**print_80ch** = Nag_FALSE, one long line of output (≤ 120 characters).

Constraint: **options**.**minor_print_level** = Nag_NoPrint or Nag_Iter.

print_deriv – Nag_DPrintType Default = Nag_D_Print

On entry: controls whether the results of any derivative checking are printed out (see also the optional parameter **options**.**verify_grad**).

If a component derivative check has been carried out, then full details will be printed if **options**.**print_deriv** = Nag_D_Print. If only a simple derivative check is requested, Nag_D_Print will produce a statement indicating failure or success. To prevent any printout from a derivative check, set **options**.**print_deriv** = Nag_D_NoPrint.

Constraint: **options**.**print_deriv** = Nag_D_NoPrint or Nag_D_Print.

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

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

crnames – char ** Default = **NULL**

On entry: if **options**.**crnames** is not **NULL** then it must point to an array of $\mathbf{n} + \mathbf{m}$ character strings with maximum string length 8, containing the names of the columns and rows (i.e., variables and constraints) of the problem. Thus, **options**.**crnames**$[j-1]$ contains the name of the jth column (variable), for $j = 1, 2, \ldots, \mathbf{n}$, and **options**.**crnames**$[\mathbf{n}+i-1]$ contains the names of the ith row (constraint), for $i = 1, 2, \ldots, \mathbf{m}$. If supplied, the names are used in the solution output (see Section 9.1 and Section 12.3).

Constraint: **options**.**crnames** = **NULL** or **strlen**(**options**.**crnames**$[i-1]$) ≤ 8, for $i = 1, 2, \ldots, \mathbf{n}+\mathbf{m}$.

obj_deriv – Nag_Boolean Default = Nag_TRUE

On entry: this argument indicates whether all elements of the objective gradient are provided in function **objfun**. If none or only some of the elements are being supplied by **objfun** then **options**.**obj_deriv** should be set to Nag_FALSE.

Whenever possible all elements should be supplied, since nag_opt_nlp_sparse (e04ugc) is more reliable and will usually be more efficient when all derivatives are exact.

If **options.obj_deriv** = Nag_FALSE, nag_opt_nlp_sparse (e04ugc) will approximate unspecified elements of the objective gradient using finite differences. The computation of finite difference approximations usually increases the total run-time, since a call to **objfun** is required for each unspecified element. Furthermore, less accuracy can be attained in the solution (see Chapter 8 of Gill *et al.* (2002), for a discussion of limiting accuracy).

At times, central differences are used rather than forward differences, in which case twice as many calls to **objfun** are needed. (The switch to central differences is not under your control.)

con_deriv – Nag_Boolean Default = Nag_TRUE

On entry: this argument indicates whether all elements of the constraint Jacobian are provided in function **confun** (or possibly directly in **a** for constant elements). If none or only some of the derivatives are being supplied then **options.con_deriv** should be set to Nag_FALSE.

Whenever possible all elements should be supplied, since nag_opt_nlp_sparse (e04ugc) is more reliable and will usually be more efficient when all derivatives are exact.

If **options.con_deriv** = Nag_FALSE, nag_opt_nlp_sparse (e04ugc) will approximate unspecified elements of the constraint Jacobian. One call to **confun** will be needed for each variable for which partial derivatives are not available. For example, if the sparsity of the constraint Jacobian has the form

$$\begin{pmatrix} * & * & & * \\ & ? & ? & \\ * & & ? & \\ & * & & * \end{pmatrix}$$

where '$*$' indicates a provided element and '?' indicates an unspecified element, nag_opt_nlp_sparse (e04ugc) will call **confun** twice: once to estimate the missing element in column 2, and again once to estimate the two missing elements in column 3. (Since columns 1 and 4 are known, they require no calls to **confun**.)

At times, central differences are used rather than forward differences, in which case twice as many calls to **confun** are needed. (The switch to central differences is not under your control.)

verify_grad – Nag_GradChk Default = Nag_SimpleCheck

On entry: specifies the level of derivative checking to be performed by nag_opt_nlp_sparse (e04ugc) on the gradient elements computed by the user-supplied functions **objfun** and **confun**. Gradients are verified at the first point that satisfies the linear constraints and the upper and lower bounds. Unspecified gradient elements are not checked, and hence they result in no overhead.

The following values are available:

Nag_NoCheck	No derivative checking is performed.
Nag_SimpleCheck	Only a cheap test is performed, requiring three calls to **objfun** and two calls to **confun**. Note that no checks are carried out if every column of the constraint gradients (Jacobian) contains a missing element.
Nag_CheckObj	Individual objective gradient elements will be checked using a reliable (but more expensive) test. If **options.print_deriv** = Nag_D_Print, a key of the form `OK` or `BAD?` indicates whether or not each element appears to be correct.
Nag_CheckCon	Individual columns or the constraint gradient (Jacobian) will be checked using a reliable (but more expensive) test. If **options.print_deriv** = Nag_D_Print, a key of the form `OK` or `BAD?` indicates whether or not each element appears to be correct.
Nag_CheckObjCon	Check both constraint and objective gradients (in that order) as described for Nag_CheckCon and Nag_CheckObj (respectively).

This component check will be made in the range specified by the optional parameters **options.obj_check_start** and **options.obj_check_stop** for the objective gradient, with default values 1

and **nonln**, respectively. For the constraint gradient the range is specified by **options.con_check_start** and **options.con_check_stop**, with default values 1 and **njnln**.

Constraint: **options.verify_grad** = Nag_NoCheck, Nag_SimpleCheck, Nag_CheckObj, Nag_CheckCon or Nag_CheckObjCon.

obj_check_start – Integer Default = 1
obj_check_stop – Integer Default = **nonln**

These options take effect only when **options.verify_grad** = Nag_CheckObj or Nag_CheckObjCon.

On entry: these arguments may be used to control the verification of gradient elements computed by the function **objfun**. For example, if the first 30 elements of the objective gradient appear to be correct in an earlier run, so that only element 31 remains questionable, it is reasonable to specify **options.obj_check_start** = 31.

Constraint: $1 \leq$ **options.obj_check_start** $\leq$ **options.obj_check_stop** $\leq$ **nonln**.

con_check_start – Integer Default = 1
con_check_stop – Integer Default = **njnln**

These options take effect only when **options.verify_grad** = Nag_CheckCon or Nag_CheckObjCon.

On entry: these arguments may be used to control the verification of the Jacobian elements computed by the function **confun**. For example, if the first 30 columns of the constraint Jacobian appeared to be correct in an earlier run, so that only column 31 remains questionable, it is reasonable to specify **options.con_check_start** = 31.

Constraint: $1 \leq$ **options.con_check_start** $\leq$ **options.con_check_stop** $\leq$ **njnln**.

f_diff_int – double Default = $\sqrt{\textbf{options.f\_prec}}$

This option does not apply when both **options.obj_deriv** and **options.con_deriv** are true.

On entry: **options.f_diff_int** defines an interval used to estimate derivatives by finite differences in the following circumstances:

(a) For verifying the objective and/or constraint gradients (see the description of the optional parameter **options.verify_grad**).

(b) For estimating unspecified elements of the objective and/or the constraint Jacobian matrix.

Using the notation $r =$ **options.f_diff_int**, a derivative with respect to x_j is estimated by perturbing that element of x to the value $x_j + r\left(1 + \left|x_j\right|\right)$, and then evaluating $f(x)$ and/or $F(x)$ (as appropriate) at the perturbed point. If the functions are well scaled, the resulting derivative approximation should be accurate to $\mathrm{O}(r)$. Judicious alteration of **options.f_diff_int** may sometimes lead to greater accuracy. See Gill *et al.* (1981) for a discussion of the accuracy in finite difference approximations.

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

c_diff_int – double Default = **options.f_prec**$^{0.33}$

This option does not apply when both **options.obj_deriv** and **options.con_deriv** are true.

On entry: **options.c_diff_int** is used near an optimal solution in order to obtain more accurate (but more expensive) estimates of gradients. This requires twice as many function evaluations as compared to using forward difference (see the optional parameter **options.f_diff_int**). Using the notation $r =$ **options.c_diff_int**, the interval used for the jth variable is $h_j = r\left(1 + \left|x_j\right|\right)$. If the functions are well scaled, the resultant gradient estimates should be accurate to $\mathrm{O}\left(r^2\right)$. The switch to central differences (not under user-control) is indicated by `C` at the end of each line of intermediate printout produced by the major iterations (see Section 5.1). The use of finite differences is discussed under the option **options.f_diff_int**.

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

crash – Nag_CrashType Default = Nag_NoCrash or Nag_CrashThreeTimes

This option does not apply when **options.start** = Nag_Warm.

On entry: the default value of **options.crash** = Nag_NoCrash if there are any nonlinear constraints, and **options.crash** = Nag_CrashThreeTimes otherwise.

If **options.start** = Nag_Cold, an internal Crash procedure is used to select an initial basis from the various rows and columns of the constraint matrix $\begin{pmatrix} A & -I \end{pmatrix}$. The value of **options.crash** determines which rows and columns of A are initially eligible for the basis, and how many times the Crash procedure is called. Columns of $-I$ are used to pad the basis where necessary. The possible choices for **options.crash** are as follows:

Nag_NoCrash	The initial basis contains only slack variables: $B = I$.
Nag_CrashOnce	The Crash procedure is called once (looking for a triangular basis in all rows and columns of A).
Nag_CrashTwice	The Crash procedure is called twice (if there are any 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 (whilst retaining the current basis for linear rows).
Nag_CrashThreeTimes	The Crash procedure is called up to three times (if there are any nonlinear constraints). The first two calls treat linear *equality* constraints and linear *inequality* constraints separately. 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 (whilst retaining the current basis for linear rows).

If **options.crash** $\neq$ Nag_NoCrash, certain slacks on inequality rows are selected for the basis first. (If **options.crash** = Nag_CrashTwice or Nag_CrashThreeTimes, 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.

Constraint: **options.crash** = Nag_NoCrash, Nag_CrashOnce, Nag_CrashTwice or Nag_CrashThreeTimes.

expand_freq – Integer Default = 10000

On entry: this option is part of the EXPAND anti-cycling procedure due to Gill *et al.* (1989), which is 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 constraints by a small amount. Suppose that the value of **options.minor_feas_tol** (see below) is δ. Over a period of **options.expand_freq** iterations, the feasibility tolerance actually used by nag_opt_nlp_sparse (e04ugc) (i.e., the *working* feasibility tolerance) increases from 0.5 to δ (in steps of $0.5\delta/$**options.expand_freq**).

For nonlinear models, the same procedure is used for iterations in which there is only one superbasic variable. (Cycling can only occur 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 the value of **options.expand_freq** helps reduce the number of slightly infeasible nonbasic basic variables (most of which are eliminated during the resetting procedure). However, it also diminishes the freedom to choose a large pivot element (see **options.pivot_tol** below).

If **options.expand_freq** = 0, the value 99999999 is used and effectively no anti-cycling procedure is invoked.

Constraint: **options.expand_freq** ≥ 0.

factor_freq – Integer Default = 50 or 100

On entry: **options**.**factor_freq** specifies the maximum number of basis changes that will occur between factorizations of the basis matrix. The default value of **options**.**factor_freq** is 50 if there are any nonlinear constraints, and 100 otherwise.

For linear problems, the basis factors are usually updated at every iteration. The default value **options**.**factor_freq** = 100 is reasonable for typical problems, particularly those that are extremely sparse and well-scaled.

When the objective function is nonlinear, fewer basis updates will occur as the solution is approached. The number of iterations between basis factorizations will therefore increase. During these iterations a test is made regularly according to the value of the optional parameter **options**.**fcheck** (see below) to ensure that the general constraints are satisfied. If necessary, the basis will be refactorized before the limit of **options**.**factor_freq** updates is reached.

Constraint: **options**.**factor_freq** ≥ 0.

fcheck – Integer Default = 60

On entry: every **options**.**fcheck**-th iteration after the most recent basis iteration, a numerical test is made to see if the current solution (x, s) satisfies the general linear constraints (including any linearized nonlinear constraints). The constraints are of the form $Ax - s = b$, where s is the set of slack variables. If the largest element of the residual vector $r = b - Ax + s$ is judged to be too large, the current basis is refactorized and the basic variables recomputed to satisfy the general constraints more accurately. If **options**.**fcheck** = 0, the value **options**.**fcheck** = 99999999 is used and effectively no checks are made.

Constraint: **options**.**fcheck** ≥ 0.

hess_freq – Integer Default = 99999999

This option only takes effect when **options**.**hess_storage** = Nag_HessianFull.

On entry: this option forces the approximate Hessian formed from **options**.**hess_freq** BFGS updates to be reset to the identity matrix upon completion of a major iteration.

Constraint: **options**.**hess_freq** > 0.

hess_update – Integer Default = 20

This option only takes effect when **options**.**hess_storage** = Nag_HessianLimited.

On entry: if **options**.**hess_storage** = Nag_HessianLimited (see below), this option defines the maximum number of pairs of Hessian update vectors that are to be used to define the quasi-Newton approximate Hessian. Once the limit of **options**.**hess_update** updates is reached, all but the diagonal elements of the accumulated updates are discarded and the process starts again. Broadly speaking, the more updates that are stored, the better the quality of the approximate Hessian. On the other hand, the more vectors that are stored, the greater the cost of each QP iteration.

The default value of **options**.**hess_update** is likely to give a robust algorithm without significant expense, but faster convergence may often be obtained with far fewer updates (e.g., **options**.**hess_update** = 5).

Constraint: **options**.**hess_update** ≥ 0.

iter_lim – Integer Default = 10000

On entry: 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 **options**.**major_iter_lim** and **options**.**minor_iter_lim** below.)

Constraint: **options**.**iter_lim** > 0.

major_iter_lim – Integer Default = 1000

On entry: specifies the maximum number of major iterations allowed before termination. It is intended to guard against an excessive number of linearizations of the nonlinear constraints. Setting

options.major_iter_lim $= 0$ and **options.print_deriv** $=$ Nag_D_Print means that the objective and constraint gradients will be checked if **options.verify_grad** $\neq$ Nag_NoCheck, but no iterations will be performed.

Constraint: **options.major_iter_lim** ≥ 0.

minor_iter_lim – Integer Default $= 500$

On entry: specifies the maximum number of iterations allowed between successive linearizations of the nonlinear constraints. A value in the range $10 \leq i \leq 50$ prevents excessive effort being expended on early major iterations, but allows later QP subproblems to be solved to completion. Note that an extra m minor iterations are allowed if the first QP subproblem to be solved starts with the all-slack basis $B = I$. (See **options.crash**.)

In general, it is unsafe to specify values as small as 1 or 2 (because even when an optimal solution has been reached, a few minor iterations may be needed for the corresponding QP subproblem to be recognised as optimal).

Constraint: **options.minor_iter_lim** ≥ 0.

part_price – Integer Default $= 1$ or 10

On entry: this option is recommended for large problems that have significantly more variables than constraints (i.e., $n \gg m$). The default value of **options.part_price** is 1 if there are any nonlinear constraints, and 10 otherwise. It reduces the work required for each 'pricing' operation (i.e., when a nonbasic variable is selected to become superbasic). The possible choices for **options.part_price** are the following.

options.part_price	**Meaning**
1	All columns of the constraint matrix $\begin{pmatrix} A & -I \end{pmatrix}$ are searched.
≥ 2	Both A and I are partitioned to give **options.part_price** roughly equal segments A_j, I_j, for $j = 1, 2, \ldots, p$ (modulo p). If the previous pricing search was successful on A_j, I_j, the next search begins on the segments A_{j+1}, I_{j+1}. 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 enter the basis. If nothing is found, the search continues on the next segments A_{j+2}, I_{j+2}, and so on.

Constraint: **options.part_price** > 0.

scale_opt – Integer Default $= 1$ or 2

On entry: the default value of **options.scale_opt** is 1 if there are any nonlinear constraints, and 2 otherwise. This option enables you to scale the variables and constraints using an iterative procedure due to Fourer (1982), which attempts to compute row scales r_i and column scales c_j such that the scaled matrix coefficients $\bar{a}_{ij} = a_{ij} \times \left(c_j / r_i\right)$ are as close as possible to unity. (The lower and upper bounds on the variables and slacks for the scaled problem are redefined as $\bar{l}_j = l_j / c_j$ and $\bar{u}_j = u_j / c_j$ respectively, where $c_j \equiv r_{j-n}$ if $j > n$.) The possible choices for **options.scale_opt** are the following.

options.scale_opt	**Meaning**
0	No scaling is performed. This is recommended if it is known that the elements of x and the constraint matrix A (along with its Jacobian) never become large (say, > 1000).

1 All linear constraints and variables are scaled. This may improve the overall efficiency of the function on some problems.

2 All constraints and variables are scaled. Also, an additional scaling is performed that takes into account columns of $\begin{pmatrix} A & -I \end{pmatrix}$ that are fixed or have positive lower bounds or negative upper bounds.

If there are any nonlinear constraints present, the scale factors depend on the Jacobian at the first point that satisfies the linear constraints and the upper and lower bounds. The setting **options.scale_opt** $= 2$ should therefore be used only if a 'good' starting point is available and the problem is not highly nonlinear.

Constraint: **options.scale_opt** $= 0$, 1 or 2.

max_sb – Integer Default $= \min(500, \mathbf{n}, \bar{n} + 1)$

This option does not apply to linear problems.

On entry: **options.max_sb** places a limit on the storage allocated for superbasic variables. Ideally, the value of **options.max_sb** should be set slightly larger than the 'number of degrees of freedom' expected at the solution.

For nonlinear problems, the number of degrees of freedom is often called the 'number of independent variables'. Normally, the value of **options.max_sb** need not be greater than $\bar{n} + 1$ (where $\bar{n} = \max(\mathbf{nonln}, \mathbf{njnln})$), but for many problems it may be considerably smaller. (This will save storage if $\bar{n}$ is very large.)

Constraint: **options.max_sb** > 0.

crash_tol – double Default $= 0.1$

On entry: this option allows the Crash procedure to ignore certain 'small' nonzero elements in the columns of A while searching for a triangular basis. If $a_{\max}$ is the largest element in the jth column, other nonzeros a_{ij} in the column are ignored if $|a_{ij}| \leq a_{\max} \times$ **options.crash_tol**.

When **options.crash_tol** > 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 earlier on some problems.

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

elastic_wt – double Default $= 1.0$ or 100.0

On entry: this option defines the initial weight γ associated with problem (8). The default value of **options.elastic_wt** is 100.0 if there are any nonlinear constraints, and 1.0 otherwise.

At any given major iteration k, elastic mode is entered if the QP subproblem is infeasible or the QP dual variables (Lagrange multipliers) are larger in magnitude than **options.elastic_wt** $\times \left(1 + \|g(x_k)\|_2\right)$, where g is the objective gradient. In either case, the QP subproblem is re-solved in elastic mode with $\gamma =$ **options.elastic_wt** $\times \left(1 + \|g(x_k)\|_2\right)$.

Constraint: **options.elastic_wt** ≥ 0.0.

f_prec – double Default $= \epsilon^{0.8}$

On entry: this option defines the *relative function precision* ϵ_R, which is intended to be a measure of the relative accuracy with which the nonlinear functions can be computed. For example, if $f(x)$ (or $F_i(x)$) is computed as 1000.56789 for some relevant x and the first 6 significant digits are known to be correct, the appropriate value for ϵ_R would be 10^{-6}.

Ideally the functions $f(x)$ or $F_i(x)$ 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 $f(x)$ (or $F_i(x)$) is computed as $1.23456789 \times 10^{-4}$ for some relevant x and the first 6 significant digits are known to be correct, the appropriate value for ϵ_R would be 10^{-10}.

The choice of ϵ_R can be quite complicated for badly scaled problems; see Chapter 8 of Gill *et al.* (1981) for a discussion of scaling techniques. The default value is appropriate for most simple functions that are computed with full accuracy.

In some cases the function values will be the result of extensive computation, possibly involving an iterative procedure that can provide few digits of precision at reasonable cost. Specifying an appropriate value of **options.f_prec** may therefore 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.

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

inf_bound – double Default $= 10^{20}$

On entry: **options.inf_bound** defines the 'infinite' bound in the definition of the problem constraints. Any upper bound greater than or equal to **options.inf_bound** will be regarded as $+\infty$ (and similarly any lower bound less than or equal to $-$**options.inf_bound** will be regarded as $-\infty$).

Constraint: **options.inf_bound** > 0.0.

linesearch_tol – double Default $= 0.9$

On entry: this option controls the accuracy with which a steplength will be located along the direction of search at each iteration. At the start of each linesearch a target directional derivative for the Lagrangian merit function is identified. The value of **options.linesearch_tol** therefore determines the accuracy to which this target value is approximated.

The default value **options.linesearch_tol** $= 0.9$ requests an inaccurate search, and is appropriate for most problems, particularly those with any nonlinear constraints.

If the nonlinear functions are cheap to evaluate, a more accurate search may be appropriate; try **options.linesearch_tol** $= 0.1$, 0.01 or 0.001. The number of major iterations required to solve the problem might decrease.

If the nonlinear functions are expensive to evaluate, a less accurate search may be appropriate. If all derivatives are available (**options.con_deriv** and **options.obj_deriv** are both true), try **options.linesearch_tol** $= 0.99$. (The number of major iterations required to solve the problem might increase, but the total number of function evaluations may decrease enough to compensate.)

If some derivatives are not available (at least one of **options.con_deriv** or **options.obj_deriv** is false), a moderately accurate search may be appropriate; try **options.linesearch_tol** $= 0.5$. Each search will (typically) require only $1 - 5$ function values, but many function calls will then be needed to estimate the missing gradients for the next iteration.

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

lu_den_tol – double Default $= 0.6$

On entry: this option defines the density tolerance used during the LU factorization of the basis matrix. 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 **options.lu_den_tol**, the Markowitz strategy for choosing pivots is terminated. The remaining matrix is then factorized using a dense LU procedure. Increasing the value of **options.lu_den_tol** towards unity may give slightly sparser LU factors, with a slight increase in factorization time.

Constraint: **options.lu_den_tol** ≥ 0.0.

lu_sing_tol – double Default $= \epsilon^{0.67}$

On entry: this option defines the singularity tolerance used to guard against ill-conditioned basis matrices. Whenever the basis is refactorized, the diagonal elements of U are tested as follows. If $|u_{jj}| \leq$ **options.lu_sing_tol** or $|u_{jj}| <$ **options.lu_sing_tol** $\times \max_i |u_{ij}|$, the jth column of the basis is replaced by the corresponding slack variable. This is most likely to occur when **options.start** $=$ Nag_Warm, or at the start of a major iteration.

In some cases, the Jacobian matrix may converge to values that make the basis exactly singular (e.g., a whole row of the Jacobian matrix could be zero at an optimal solution). Before exact singularity occurs, the basis could become very ill-conditioned and the optimization could progress very slowly (if at all). Setting **options.lu_sing_tol** $= 0.00001$ (say) may therefore help cause a judicious change of basis in such situations.

Constraint: **options.lu_sing_tol** > 0.0.

lu_factor_tol – double Default $= 5.0$ or 100.0
lu_update_tol – double Default $= 5.0$ or 10.0

On entry: **options.lu_factor_tol** and **options.lu_update_tol** affect the stability and sparsity of the basis factorization $B = LU$, during refactorization and updates respectively. The default values are **options.lu_factor_tol** $=$ **options.lu_update_tol** $= 5.0$ if there are any nonlinear constraints, and **options.lu_factor_tol** $= 100.0$ and **options.lu_update_tol** $= 10.0$ otherwise.

The lower triangular matrix L can be seen as a product of matrices of the form

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

where the multipliers μ satisfy $|\mu| <$ **options.lu_factor_tol** during refactorization or $|\mu| <$ **options.lu_update_tol** during update. The default values of **options.lu_factor_tol** and **options.lu_update_tol** usually strike a good compromise between stability and sparsity. Smaller values of **options.lu_factor_tol** and **options.lu_update_tol** favour stability, while larger values favour sparsity. For large and relatively dense problems, setting **options.lu_factor_tol** to 10.0 or 5.0 (say) may give a marked improvement in sparsity without impairing stability to a serious degree. Note that for problems involving band matrices it may be necessary to reduce **options.lu_factor_tol** and/or **options.lu_update_tol** in order to achieve stability.

Constraints:

options.lu_factor_tol ≥ 1.0;
options.lu_update_tol ≥ 1.0.

major_feas_tol – double Default $= \sqrt{\epsilon}$

On entry: this option specifies how accurately the nonlinear constraints should be satisfied. The default value is appropriate when the linear and nonlinear constraints contain data to approximately that accuracy. A larger value may be appropriate if some of the problem functions are known to be of low accuracy.

Let *rowerr* be defined as the maximum nonlinear constraint violation normalized by the size of the solution. It is required to satisfy

$$rowerr = \max_i \frac{viol_i}{\|(x,s)\|} \quad \leq \quad \textbf{options.major\_feas\_tol},$$

where $viol_i$ is the violation of the ith nonlinear constraint.

Constraint: **options.major_feas_tol** $> \epsilon$.

major_opt_tol – double Default $= \sqrt{\epsilon}$

On entry: this option specifies the final accuracy of the dual variables. If nag_opt_nlp_sparse (e04ugc) terminates with **fail.code** $=$ NE_NOERROR, a primal and dual solution (x, s, π) will have been computed such that

$$maxgap = \max_j \frac{gap_j}{\|\pi\|} \quad \leq \quad \textbf{options.major\_opt\_tol},$$

where gap_j is an estimate of the complementarity gap for the jth variable and $\|\pi\|$ is a measure of the size of the QP dual variables (or Lagrange multipliers) given by

$$\|\pi\| = \max\left(\frac{\sigma}{\sqrt{m}}, 1\right), \qquad \text{where} \quad \sigma = \sum_{i=1}^{m} |\pi_i|.$$

It is included to make the tests independent of a scale factor on the objective function. Specifically, gap_j is 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 element of the objective gradient and a_j is the associated column of the constraint matrix $\begin{pmatrix} A & -I \end{pmatrix}$:

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

Constraint: **options.major_opt_tol** > 0.0.

major_step_lim – double Default $= 2.0$

On entry: this option 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 in the interval $0 < \alpha \leq \beta$, where $\beta = 1$ if there are any nonlinear constraints, or the step to the nearest upper or lower bound on x if all the constraints are linear. Normally, the first step attempted is $\alpha_1 = \min(1, \beta)$.

In some cases, such as $f(x) = ae^{bx}$ or $f(x) = ax^b$, even a moderate change in the elements of x can lead to floating-point overflow. The optional parameter **options.major_step_lim** is therefore used to define a step limit $\bar{\beta}$ given by

$$\bar{\beta} = \frac{\textbf{options.major\_step\_lim}\left(1 + \|x\|_2\right)}{\|p\|_2},$$

where p is the search direction and the first evaluation of $f(x)$ is made at the (potentially) smaller step length $\alpha_1 = \min\left(1, \bar{\beta}, \beta\right)$.

Wherever possible, upper and lower bounds on x should be used to prevent evaluation of nonlinear functions at meaningless points. **options.major_step_lim** provides an additional safeguard. The default value **options.major_step_lim** $= 2.0$ should not affect progress on well-behaved functions, but values such as **options.major_step_lim** $= 0.1$ or 0.01 may be helpful when rapidly varying functions are present. If a small value of **options.major_step_lim** is selected, a 'good' starting point may be required. An important application is to the class of nonlinear least squares problems.

Constraint: **options.major_step_lim** > 0.0.

minor_feas_tol – double Default $= \sqrt{\epsilon}$

On entry: this option attempts to ensure that all variables eventually satisfy their upper and lower bounds to within the tolerance **options.minor_feas_tol**. Since this includes slack variables, general linear constraints should also be satisfied to within **options.minor_feas_tol**. Note that feasibility with respect to nonlinear constraints is judged by the value of **options.major_feas_tol** and not by **options.minor_feas_tol**.

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

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

Nonlinear functions will only be evaluated at points that satisfy the bounds and linear constraints. If there are regions where a function is undefined, every effort should be made to eliminate these regions from the problem. For example, if $f(x_1, x_2) = \sqrt{x_1} + \log(x_2)$, it is essential to place lower bounds on both x_1 and x_2. If the value **options.minor_feas_tol** $= 10^{-6}$ is used, the bounds $x_1 \geq 10^{-5}$ and $x_2 \geq 10^{-4}$ might be appropriate. (The log singularity is more serious; in general, you should attempt to keep x as far away from singularities as possible.)

In reality, **options.minor_feas_tol** is used 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 and the function is then in *elastic mode* thereafter (with only the linearized nonlinear constraints defined to be elastic). (See also **options.elastic_wt**.)

Constraint: **options.minor_feas_tol** $> \epsilon$.

minor_opt_tol – double Default $= \sqrt{\epsilon}$

On entry: this option is used to judge optimality for each QP subproblem. Let the QP reduced gradients be $d_j = g_j - \pi^{\mathrm{T}} a_j$, where g_j is the jth element of the QP gradient, a_j is the associated column of the QP constraint matrix and π is the set of QP dual variables.

By construction, the reduced gradients for basic variables are always zero. The QP subproblem will be declared optimal if the reduced gradients for nonbasic variables at their upper or lower bounds satisfy

$$\frac{d_j}{\|\pi\|} \geq -\textbf{options.minor\_opt\_tol} \quad \text{or} \quad \frac{d_j}{\|\pi\|} \leq \textbf{options.minor\_opt\_tol}$$

respectively, and if $\frac{|d_j|}{\|\pi\|} \leq$ **options.minor_opt_tol** for superbasic variables.

Note that $\|\pi\|$ is a measure of the size of the dual variables. It is included to make the tests independent of a scale factor on the objective function. (The value of $\|\pi\|$ actually used is defined in the description of the optional parameter **options.major_opt_tol**.)

If the objective is scaled down to be very *small*, the optimality test reduces to comparing d_j against **options.minor_opt_tol**.

Constraint: **options.minor_opt_tol** > 0.0.

nz_coef – double Default $= 5.0$

This option is ignored if **options.hess_storage** = Nag_HessianFull.

On entry: **options.nz_coef** defines how much memory is initially allocated for the basis factors: by default, nag_opt_nlp_sparse (e04ugc) allocates approximatively **nnz** $\times$ **options.nz_coef** reals and $2 \times$ **nnz** $\times$ **options.nz_coef** integers in order to compute and store the basis factors. If at some point this appears not to be enough, an internal warm restart with more memory is automatically attempted, so that nag_opt_nlp_sparse (e04ugc) should complete anyway. Thus this option generally does not need to be modified.

However, if a lot of memory is available, it is possible to increase the value of **options.nz_coef** such as to limit the number of compressions of the work space and possibly avoid internal restarts. On the other hand, for large problems where memory might be critical, decreasing the value of **options.nz_coef** can sometimes save some memory.

Constraint: **options.nz_coef** ≥ 1.0.

pivot_tol – double Default $= \epsilon^{0.67}$

On entry: this option is used during the solution of QP subproblems 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 specified search direction p, a 'ratio test' is used to determine which element 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 **options.pivot_tol**.

It is common in practice for two (or more) variables to reach a bound at essentially the same time. In such cases, the optional parameter **options.minor_feas_tol** provides some freedom to maximize the pivot element and thereby improve numerical stability. Excessively *small* values of **options.minor_feas_tol** should therefore not be specified. To a lesser extent, the optional parameter

options.expand_freq also provides some freedom to maximize the pivot element. Excessively *large* values of **options.expand_freq** should therefore not be specified.

Constraint: **options.pivot_tol** > 0.0.

scale_tol – double Default $= 0.9$

On entry: this option is used to control the number of scaling passes to be made through the constraint matrix A. At least 3 (and at most 10) passes will be made. More precisely, let a_p denote the largest column ratio (i.e., $\frac{\text{'biggest' element}}{\text{'smallest' element}}$ in some sense) after the pth scaling pass through A. The scaling procedure is terminated if $a_p \geq a_{p-1} \times$ **options.scale_tol** for some $p \geq 3$. Thus, increasing the value of **options.scale_tol** from 0.9 to 0.99 (say) will probably increase the number of passes through A.

Constraint: $0.0 <$ **options.scale_tol** < 1.0.

unbounded_obj – double Default $= 10^{15}$
inf_step – double Default $= \max(\textbf{options.inf\_bound}, 10^{20})$

On entry: these options are intended to detect unboundedness in nonlinear problems. During the linesearch, the objective function f is evaluated at points of the form $x + \alpha p$, where x and p are fixed and α varies. If $|f|$ exceeds **options.unbounded_obj** or α exceeds **options.inf_step**, the iterations are terminated and the function returns with **fail.code** = NE_MAYBE_UNBOUNDED.

If singularities are present, unboundedness in $f(x)$ may manifest itself by a floating-point overflow during the evaluation of $f(x + \alpha p)$, before the test against **options.unbounded_obj** can be made.

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

Constraints:

options.unbounded_obj > 0.0;
options.inf_step > 0.0.

violation_limit – double Default $= 10.0$

On entry: this option defines an absolute limit on the magnitude of the maximum constraint violation after the linesearch. Upon completion of the linesearch, the new iterate x_{k+1} satisfies the condition

$$v_i(x_{k+1}) \leq \textbf{options.violation\_limit} \times \max(1, v_i(x_0)),$$

where x_0 is the point at which the nonlinear constraints are first evaluated and $v_i(x)$ is the ith nonlinear constraint violation $v_i(x) = \max(0, l_{i-F}i - F_i(x), F_i(x) - u_i)$.

The effect of the violation limit is to restrict the iterates to lie in an *expanded* feasible region whose size depends on the magnitude of **options.violation_limit**. This makes it possible to keep the iterates within a region where the objective function is expected to be well-defined and bounded below (or above in the case of maximization). If the objective function is bounded below (or above in the case of maximization) for all values of the variables, then **options.violation_limit** may be any large positive value.

Constraint: **options.violation_limit** > 0.0.

deriv_linesearch – Nag_Boolean Default $=$ Nag_TRUE

On entry: at each major iteration, a linesearch is used to improve the value of the Lagrangian merit function (6). The default linesearch uses safeguarded cubic interpolation and requires both function and gradient values in order to compute estimates of the step α_k. If some analytic derivatives are not provided or **options.deriv_linesearch** = Nag_FALSE is specified, a linesearch based upon safeguarded quadratic interpolation (which does not require the evaluation or approximation of any gradients) is used instead.

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

If **options.deriv_linesearch** = Nag_FALSE is selected, nag_opt_nlp_sparse (e04ugc) signals the evaluation of the linesearch by calling **objfun** and **confun** with **comm→flag** = 0. Once the linesearch is complete, the nonlinear functions are re-evaluated with **comm→flag** = 2. If the potential savings offered by a nonderivative linesearch are to be fully realised, it is essential that **objfun** and **confun** be coded so that no derivatives are computed when **comm→flag** = 0.

Constraint: **options.deriv_linesearch** = Nag_TRUE or Nag_FALSE.

feas_exit – Nag_Boolean Default = Nag_FALSE

This option is ignored if the value of **options.major_iter_lim** is exceeded, or the linear constraints are infeasible.

On entry: if termination is about to occur at a point that does not satisfy the nonlinear constraints and **options.feas_exit** = Nag_TRUE is selected, this option requests that additional iterations be performed in order to find a feasible point (if any) for the nonlinear constraints. This involves solving a feasible point problem in which the objective function is omitted.

Otherwise, this option requests no additional iterations be performed.

Constraint: **options.feas_exit** = Nag_TRUE or Nag_FALSE.

hess_storage – Nag_HessianType Default = Nag_HessianFull or Nag_HessianLimited

On entry: this option specifies the method for storing and updating the quasi-Newton approximation to the Hessian of the Lagrangian function. The default is Nag_HessianFull if the number of nonlinear variables $\bar{n}$ (= max(**nonln**, **njnln**)) < 75, and Nag_HessianLimited otherwise.

If **options.hess_storage** = Nag_HessianFull, the approximate Hessian is treated as a dense matrix, and BFGS quasi-Newton updates are applied explicitly. This is most efficient when the total number of nonlinear variables is not too large (say, $\bar{n} < 75$). In this case, the storage requirement is fixed and you can expect one-step Q-superlinear convergence to the solution.

options.hess_storage = Nag_HessianLimited should only be specified when $\bar{n}$ 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.)

Note that if **options.hess_freq** = 20 is used in conjunction with **options.hess_storage** = Nag_HessianFull, the effect will be similar to using **options.hess_storage** = Nag_HessianLimited in conjunction with **options.hess_update** = 20, except that the latter will retain the current diagonal during resets.

Constraint: **options.hess_storage** = Nag_HessianLimited or Nag_HessianFull.

direction – Nag_DirectionType Default = Nag_Minimize

On entry: if **options.direction** = Nag_FeasiblePoint, nag_opt_nlp_sparse (e04ugc) attempts to find a feasible point (if any) for the nonlinear constraints by omitting the objective function. It can also be used to check whether the nonlinear constraints are feasible.

Otherwise, **options.direction** specifies the direction of optimization. It applies to both linear and nonlinear terms (if any) in the objective function. Note that if two problems are the same except that one minimizes $f(x)$ and the other maximizes $-f(x)$, their solutions will be the same but the signs of the dual variables π_i and the reduced gradients d_j will be reversed.

Constraint: **options.direction** = Nag_FeasiblePoint, Nag_Minimize or Nag_Maximize.

state – Integer * Default memory = **n** + **m**

On entry: **options.state** need not be set if the default option of **options.start** = Nag_Cold is used as **n** + **m** values of memory will be automatically allocated by nag_opt_nlp_sparse (e04ugc).

If the optional parameter **options.start** = Nag_Warm has been chosen, **options.state** must point to a minimum of **n** + **m** elements of memory. This memory will already be available if the **options** structure has been used in a previous call to nag_opt_nlp_sparse (e04ugc) from the calling program, with

options.start = Nag_Cold and the same values of **n** and **m**. If a previous call has not been made you must allocate sufficient memory.

If you supply a **options.state** vector and **options.start** = Nag_Cold, then the first **n** elements of **options.state** must specify the initial states of the problem variables. (The slacks s need not be initialized.) An internal Crash procedure is then used to select an initial basis matrix B. The initial basis matrix will be triangular (neglecting certain small elements in each column). It is chosen from various rows and columns of $\begin{pmatrix} A & -I \end{pmatrix}$. Possible values for **options.state**$[j-1]$, for $j = 1, 2, \ldots,$ **n**, are:

options.state$[j-1]$	**State of xs**$[j-1]$ **during Crash procedure**
0 or 1	Eligible for the basis
2	Ignored
3	Eligible for the basis (given preference over 0 or 1)
4 or 5	Ignored

If nothing special is known about the problem, or there is no wish to provide special information, you may set **options.state**$[j-1] = 0$ (and **xs**$[j-1] = 0.0$), for $j = 1, 2, \ldots,$ **n**. All variables will then be eligible for the initial basis. Less trivially, to say that the jth variable will probably be equal to one of its bounds, you should set **options.state**$[j-1] = 4$ and **xs**$[j-1] =$ **bl**$[j-1]$ or **options.state**$[j-1] = 5$ and **xs**$[j-1] =$ **bu**$[j-1]$ as appropriate.

Following the Crash procedure, variables for which **options.state**$[j-1] = 2$ are made superbasic. Other variables not selected for the basis are then made nonbasic at the value **xs**$[j-1]$ if **bl**$[j-1] \leq$ **xs**$[j-1] \leq$ **bu**$[j-1]$, or at the value **bl**$[j-1]$ or **bu**$[j-1]$ closest to **xs**$[j-1]$.

When **options.start** = Nag_Warm, **options.state** and **xs** must specify the initial states and values, respectively, of the variables and slacks (x, s). If nag_opt_nlp_sparse (e04ugc) has been called previously with the same values of **n** and **m**, **options.state** already contains satisfactory information.

Constraints:

if **options.start** = Nag_Cold, $0 \leq$ **options.state**$[j-1] \leq 5$, for $j = 1, 2, \ldots,$ **n**;
if **options.start** = Nag_Warm, $0 \leq$ **options.state**$[j-1] \leq 3$, for $j = 1, 2, \ldots,$ **n** + **m**.

On exit: the final states of the variables and slacks (x, s). The significance of each possible value of **options.state** is as follows:

options.state$[j-1]$	**State of variable** j	**Normal value of xs**$[j-1]$
0	Nonbasic	**bl**$[j-1]$
1	Nonbasic	**bu**$[j-1]$
2	Superbasic	Between **bl**$[j-1]$ and **bu**$[j-1]$
3	Basic	Between **bl**$[j-1]$ and **bu**$[j-1]$

If the problem is feasible (i.e., **ninf** = 0), basic and superbasic variables may be outside their bounds by as much as the optional parameter **options.minor_feas_tol**. Note that unless the optional parameter **options.scale_opt** = 0, **options.minor_feas_tol** applies to the variables of the scaled problem. In this case, the variables of the original problem may be as much as 0.1 outside their bounds, but this is unlikely unless the problem is very badly scaled.

Very occasionally some nonbasic variables may be outside their bounds by as much as **options.minor_feas_tol**, and there may be some nonbasic variables for which **xs**$[j-1]$ lies strictly between its bounds.

If the problem is infeasible (i.e., **ninf** > 0), some basic and superbasic variables may be outside their bounds by an arbitrary amount (bounded by **sinf** if scaling was not used (**options.scale_opt** = 0).

lambda – double * Default memory = **n** + **m**

On entry: if **options.start** = Nag_Cold, you do not need to provide memory for **options.lambda**, as **n** + **m** values of memory will be automatically allocated by nag_opt_nlp_sparse (e04ugc). This is the recommended method of use of **options.lambda**. However you may supply memory from the calling program.

If the option **options.start** = Nag_Warm has been chosen, **options.lambda** must point to a minimum of $\mathbf{n} + \mathbf{m}$ elements of memory. This memory will already be available if the **options** structure has been used in a previous call to nag_opt_nlp_sparse (e04ugc) from the calling program, with **options.start** = Nag_Cold and the same values of **n** and **m**. If a previous call has not been made, you must allocate sufficient memory.

When a 'warm start' is chosen **options.lambda**$[j-1]$ must contain a multiplier estimate for each nonlinear constraint for $j = \mathbf{n}+1, \mathbf{n}+2, \ldots, \mathbf{n}+\mathbf{ncnln}$. The remaining elements need not be set. If nothing is known about the problem, or there is no wish to provide special information, you may set **options.lambda**$[j-1] = 0$ for $j = \mathbf{n}+1, \mathbf{n}+2, \ldots, \mathbf{n}+\mathbf{ncnln}$.

On exit: a set of Lagrange multipliers for the bound constraints on the variables (*reduced costs*) and the general constraints (*shadow costs*). More precisely, the first **n** elements contain the multipliers for the bound constraints on the variables, the next **ncnln** elements contain the multipliers for the nonlinear constraints $F(x)$ (if any) and the next $\mathbf{m} - \mathbf{ncnln}$ elements contain the multipliers for the linear constraints Gx and the free row (if any).

iter – Integer

On exit: the total number of minor iterations (summed over all major iterations).

major_iter – Integer

On exit: the number of major iterations that have been performed in nag_opt_nlp_sparse (e04ugc).

nsb – Integer

On entry: the number of superbasic variables. It need not be specified if **options.start** = Nag_Cold but must retain its value from a previous call when **options.start** = Nag_Warm.

Constraint: if **options.start** = Nag_Warm, **options.nsb** ≥ 0.

On exit: the final number of superbasic variables.

nf – Integer

On exit: the number of calls to **objfun**.

ncon – Integer

On exit: the number of calls to **confun**.

12.3 Description of Printed Output

This section describes the intermediate printout and final printout produced by nag_opt_nlp_sparse (e04ugc). The level of printed output can be controlled with the structure members **options.list**, **options.print_deriv**, **options.print_level**, **options.minor_print_level**, **options.print_80ch**, and **options.outfile** (see Section 12.2). If **options.list** = Nag_TRUE then the argument values to nag_opt_nlp_sparse (e04ugc) are listed, followed by the result of any derivative check when **options.print_deriv** = Nag_D_Print. The printout of results is then governed by the values of **options.print_80ch**, **options.print_level** and **options.minor_print_level**. The default of **options.print_level** = Nag_Soln_Iter, **options.minor_print_level** = Nag_NoPrint, and **options.print_80ch** = Nag_TRUE produces a single line of output at each major iteration and the final result (see Section 5.1). This section describes all of the possible other levels of results printout available from nag_opt_nlp_sparse (e04ugc).

If a simple derivative check, **options.verify_grad** = Nag_SimpleCheck, is requested then a statement indicating success or failure is given. The largest error found in the objective and the constraint Jacobian are also output.

When a component derivative check (see the optional parameter **options.verify_grad** in Section 12.2) is selected, the element with the largest relative error is identified for the objective and the constraint Jacobian.

If **options.print_deriv** = Nag_D_Print then the following results are printed for each component:

`x[j-1]` the element of x.

`dx[j-1]` the finite difference interval.

`Jacobian value` the nonlinear Jacobian element.

`g[j-1]` the objective gradient element.

`Difference approx.` the finite difference approximation.

The indicator, `OK` or `BAD?`, states whether the derivative provided and the finite difference approximation are in agreement. If the derivatives are believed to be in error nag_opt_nlp_sparse (e04ugc) will exit with **fail** set to either NE_CON_DERIV_ERRORS or NE_OBJ_DERIV_ERRORS, depending on whether the error was detected in the constraint Jacobian or in the objective gradient.

When **options**.**print_level** = Nag_Iter, Nag_Soln_Iter or Nag_Soln_Iter_Full, and **options**.**print_80ch** = Nag_FALSE, the following line of intermediate printout (≤ 120 characters) is sent at every major iteration to **options**.**outfile**. Unless stated otherwise, the values of the quantities printed are those in effect *on completion* of the given iteration.

`Major` is the major iteration count.

`Minor` is the number of minor iterations required by the feasibility and optimality phases of the QP subproblem. Generally, `Minor` 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 taken along the computed search direction. On reasonably well-behaved problems, the unit step will be taken as the solution is approached.

`nObj` is the number of times **objfun** has been called to evaluate the nonlinear part of the objective function. Evaluations needed for the estimation of the gradients by finite differences are not included. `nObj` is printed as a guide to the amount of work required for the linesearch.

`nCon` is the number of times **confun** has been called to evaluate the nonlinear constraint functions (not printed if **ncnln** is zero).

`Merit` is the value of the augmented Lagrangian merit function (6) at the current iterate. This function will decrease at each iteration unless it was necessary to increase the penalty parameters (see Section 11.1). As the solution is approached, `Merit` will converge to the value of the objective function at the solution.

In elastic mode (see Section 11.2), the merit function is a composite function involving the constraint violations weighted by the value of the optional parameter **options**.**elastic_wt** (default value $= 1.0$ or 100.0).

If there are no nonlinear constraints present, this entry contains `Objective`, the value of the objective function $f(x)$. In this case, $f(x)$ will decrease monotonically to its optimal value.

`Feasibl` is the value of *rowerr*, the largest element of the scaled nonlinear constraint residual vector defined in the description of the optional parameter **options**.**major_feas_tol**. The solution is regarded as 'feasible' if `Feasibl` is less than (or equal to) **options**.**major_feas_tol** (default value $= \sqrt{\epsilon}$). `Feasibl` will be approximately zero in the neighbourhood of a solution.

If there are no nonlinear constraints present, all iterates are feasible and this entry is not printed.

`Optimal` is the value of *maxgap*, the largest element of the maximum complementarity gap vector defined in the description of the optional parameter **options**.**major_opt_tol**. The Lagrange multipliers are regarded as 'optimal' if `Optimal` is less than (or equal to) **options**.**major_opt_tol** (default value $= \sqrt{\epsilon}$). `Optimal` will be approximately zero in the neighbourhood of a solution.

`nS` is the current number of superbasic variables.

`Penalty` is the Euclidean norm of the vector of penalty parameters used in the augmented Lagrangian function (not printed if **ncnln** is zero).

`LU` is the number of nonzeros representing the basis factors L and U on completion of the QP subproblem.

If there are nonlinear constraints present, the basis factorization $B = LU$ is computed at the start of the first minor iteration. At this stage, `LU` = `lenL` + `lenU`, where `lenL` is the number of subdiagonal elements in the columns of a lower triangular matrix and `lenU` 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, the value of `LU` may fluctuate up or down (but in general will tend to increase). As the solution is approached and the number of minor iterations required to solve each QP subproblem decreases towards zero, `LU` will reflect the number of nonzeros in the LU factors at the start of each QP subproblem.

If there are no nonlinear constraints present, refactorization is subject only to the value of the optional parameter **options.factor_freq** (default value = 50 or 100) and hence `LU` will tend to increase between factorizations.

`Swp` is the number of columns of the basis matrix B that were swapped with columns of S in order to improve the condition number of B (not printed if **ncnln** is zero). The swaps are determined by an LU factorization of the rectangular matrix $B_S = (B \quad S)^{\mathrm{T}}$, with stability being favoured more than sparsity.

`Cond Hz` is an estimate of the condition number of the reduced Hessian of the Lagrangian (not printed if **ncnln** and **nonln** are both zero). It is the square of the ratio between the largest and smallest diagonal elements of the upper triangular matrix R. This constitutes a lower bound on the condition number of the matrix $R^{\mathrm{T}}R$ that approximates the reduced Hessian. The larger this number, the more difficult the problem.

`PD` is a two-letter indication of the status of the convergence tests involving the feasibility and optimality of the iterates defined in the descriptions of the optional parameters **options.major_feas_tol** and **options.major_opt_tol**. Each letter is `T` if the test is satisfied, and `F` otherwise. The tests indicate whether the values of `Feasibl` and `Optimal` are sufficiently small. For example, `TF` or `TT` is printed if there are no nonlinear constraints present (since all iterates are feasible).

`M` is printed if an extra evaluation of **objfun** and **confun** was needed in order to define an acceptable positive definite quasi-Newton update to the Hessian of the Lagrangian. This modification is only performed when there are nonlinear constraints present.

`m` is printed if, in addition, it was also necessary to modify the update to include an augmented Lagrangian term.

`s` is printed if a self-scaled BFGS (Broyden–Fletcher–Goldfarb–Shanno) update was performed. This update is always used when the Hessian approximation is diagonal, and hence always follows a Hessian reset.

`S` is printed if, in addition, it was also necessary to modify the self-scaled update in order to maintain positive-definiteness.

`n` is printed if no positive definite BFGS update could be found, in which case the approximate Hessian is unchanged from the previous iteration.

`r` is printed if the approximate Hessian was reset after 10 consecutive major iterations in which no BFGS update could be made. The diagonal elements of the approximate Hessian are retained if at least one update has been performed since the last reset. Otherwise, the approximate Hessian is reset to the identity matrix.

`R` is printed if the approximate Hessian has been reset by discarding all but its diagonal elements. This reset will be forced periodically by the values of the optional parameters **options.hess_freq** (default value = 99999999) and

options.hess_update (default value $= 20$). However, it may also be necessary to reset an ill-conditioned Hessian from time to time.

`l` is printed if the change in the variables was limited by the value of the optional parameter **options.major_step_lim** (default value $= 2.0$). If this output occurs frequently during later iterations, it may be worthwhile increasing the value of **options.major_step_lim**.

`c` is printed if central differences have been used to compute the unknown elements 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.

`u` is printed if the QP subproblem was unbounded.

`t` is printed if the minor iterations were terminated because the number of iterations specified by the value of the optional parameter **options.minor_iter_lim** (default value $= 500$) was reached.

`i` is printed if the QP subproblem was infeasible when the function was not in elastic mode. 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 (8) (see Section 11.2). It is also printed if the minimizer of the elastic subproblem does not satisfy the linearized constraints when the function is already in elastic mode. (In this case, a feasible point for the usual QP subproblem may or may not exist.)

`w` is printed if a weak solution of the QP subproblem was found.

When **options.minor_print_level** = Nag_Iter and **options.print_80ch** = Nag_TRUE, the following line of intermediate printout (≤ 80 characters) is sent at every minor iteration to **options.outfile**. Unless stated otherwise, the values of the quantities printed are those in effect *on completion* of the given iteration.

`Itn` is the iteration count.

`Step` is the step taken along the computed search direction.

`Ninf` is the number of infeasibilities. This will not increase unless the iterations are in elastic mode. `Ninf` will be zero during the optimality phase.

`Sinf` is the value of the sum of infeasibilities if `Ninf` is nonzero. This will be zero during the optimality phase.

`Objective` is the value of the current QP objective function when `Ninf` is zero and the iterations are not in elastic mode. The switch to elastic mode is indicated by a change in the heading to `Composite Obj` (see below).

`Composite Obj` is the value of the composite objective function (9) when the iterations are in elastic mode. This function will decrease monotonically at each iteration.

`Norm rg` is the Euclidean norm of the reduced gradient of the QP objective function. During the optimality phase, this norm will be approximately zero after a unit step.

When **options.minor_print_level** = Nag_Iter and **options.print_80ch** = Nag_FALSE, the following line of intermediate printout (≤ 120 characters) is sent at every minor iteration to **options.outfile**. Unless stated otherwise, the values of the quantities printed are those in effect *on completion* of the given iteration.

In the description below, a 'pricing' operation is defined to be the process by which a nonbasic variable is selected to become superbasic (in addition to those already in the superbasic set). If the problem is purely linear, the variable selected will usually become basic immediately (unless it happens to reach its opposite bound and return to the nonbasic set).

`Itn` is the iteration count.

`pp` is the partial price indicator. The variable selected by the last pricing operation came from the `pp`-th partition of A and $-I$. Note that `pp` is reset to zero whenever the basis is refactorized.

`dj` is the value of the reduced gradient (or reduced cost) for the variable selected by the pricing operation at the start of the current iteration.

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

`-SBS` is the variable chosen to leave the superbasic set. It has become basic if the entry under `-B` is nonzero; otherwise it has become nonbasic.

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

`-B` is the variable removed from the basis (if any) to swap with a slack variable made superbasic by the latest pricing operation. The swap is done to ensure that there are no superbasic slacks.

`Step` is the value of the step length α taken along the current search direction p. The variables x have just been changed to $x + \alpha p$. If a variable is made superbasic during the current iteration (i.e., `+SBS` is positive), `Step` will be the step to the nearest bound. During the optimality phase, the step can be greater than unity only if the reduced Hessian is not positive definite.

`Pivot` is the rth element of a vector y satisfying $By = a_q$ whenever a_q (the qth column of the constraint matrix $\begin{pmatrix} A & -I \end{pmatrix}$) replaces the rth column of the basis matrix B. Wherever possible, `Step` is chosen so as to avoid extremely small values of `Pivot` (since they may cause the basis to be nearly singular). In extreme cases, it may be necessary to increase the value of the optional parameter **options.pivot_tol** (default value $= \epsilon^{0.67}$) to exclude very small elements of y from consideration during the computation of `Step`.

`Ninf` is the number of infeasibilities. This will not increase unless the iterations are in elastic mode. `Ninf` will be zero during the optimality phase.

`Sinf/Objective` is the value of the current objective function. If x is infeasible, `Sinf` gives the value of the sum of infeasibilities at the start of the current iteration. It will usually decrease at each nonzero value of `Step`, but may occasionally increase if the value of `Ninf` decreases by a factor of 2 or more. However, in elastic mode this entry gives the value of the composite objective function (9), which will decrease monotonically at each iteration. If x is feasible, `Objective` is the value of the current QP objective function.

`L` is the number of nonzeros in the basis factor L. Immediately after a basis factorization $B = LU$, this entry contains `lenL`. Further nonzeros are added to `L` when various columns of B are later replaced. (Thus, `L` increases monotonically.)

`U` is the number of nonzeros in the basis factor U. Immediately after a basis factorization $B = LU$, this entry contains `lenU`. As columns of B are replaced, the matrix U is maintained explicitly (in sparse form). The value of `U` may fluctuate up or down; in general, it will tend to increase.

`Ncp` is the number of compressions required to recover workspace in the data structure for U. This includes the number of compressions needed during the previous basis factorization. Normally, `Ncp` should increase very slowly. If it does not, nag_opt_nlp_sparse (e04ugc) will attempt to expand the internal workspace allocated for the basis factors.

The following items are printed only if the problem is nonlinear or the superbasic set is non-empty (i.e., if the current solution is nonbasic).

`Norm rg` is the Euclidean norm of the reduced gradient at the start of the current iteration. During the optimality phase, this norm will be approximately zero after a unit step.

`nS` is the current number of superbasic variables.

`Cond Hz` is an estimate of the condition number of the reduced Hessian of the Lagrangian (not printed if **ncnln** and **nonln** are both zero). It is the square of the ratio between the largest and smallest diagonal elements of an upper triangular matrix R. This constitutes a lower bound on the condition number of the matrix $R^{\mathrm{T}}R$ that approximates the reduced Hessian. The larger this number, the more difficult the problem.

When **options**.**print_level** = Nag_Soln_Iter_Full, the following lines of intermediate printout (≤ 120 characters) are sent to **options**.**outfile** whenever the matrix B or $B_S = (B \quad S)^{\mathrm{T}}$ is factorized. Gaussian elimination is used to compute a sparse LU factorization of B or B_S, where PLP^{T} is a lower triangular matrix and PUQ is an upper triangular matrix for some permutation matrices P and Q. The factorization is stabilized in the manner described under the optional parameter **options**.**lu_factor_tol** (default value $= 5.0$ or 100.0).

Note that B_S may be factorized at the beginning of just some of the major iterations. It is immediately followed by a factorization of B itself. Note also that factorizations can occur during the solution of a QP problem.

`Factorize` is the factorization count.

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

Code	Meaning
0	First LU factorization.
1	The number of updates reached the value of the optional parameter **options**.**factor_freq** (default value $= 50$ or 100).
2	The number of nonzeros in the updated factors has increased significantly.
7	Not enough storage to update factors.
10	Row residuals too large (see the description for the optional parameter **options**.**fcheck**).
11	Ill-conditioning has caused inconsistent results.

`Iteration` is the iteration count.

`Nonlinear` is the number of nonlinear variables in the current basis B (not printed if B_S is factorized).

`Linear` is the number of linear variables in B (not printed if B_S is factorized).

`Slacks` is the number of slack variables in B (not printed if B_S is factorized).

`Elems` is the number of nonzeros in B (not printed if B_S is factorized).

`Density` is the percentage nonzero density of B (not printed if B_S is factorized). More precisely, $\texttt{Density} = 100 \times \texttt{Elems}/(\texttt{Nonlinear} + \texttt{Linear} + \texttt{Slacks})^2$.

`Compressns` is the number of times the data structure holding the partially factorized matrix needed to be compressed, in order to recover unused workspace. Ideally, it should be zero.

`Merit` 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 `m` such quantities. It gives an indication of how much work was required to preserve sparsity during the factorization.

`lenL` is the number of nonzeros in L.

`lenU` is the number of nonzeros in U.

`Increase` is the percentage increase in the number of nonzeros in L and U relative to the number of nonzeros in B. More precisely, $\texttt{Increase} = 100 \times (\texttt{lenL} + \texttt{lenU} - \texttt{Elems})/\texttt{Elems}$.

`m` is the number of rows in the problem. Note that $\texttt{m} = \texttt{Ut} + \texttt{Lt} + \texttt{bp}$.

`Ut` is the number of triangular rows of B at the top of U.

`d1` is the number of columns remaining when the density of the basis matrix being factorized reached 0.3.

`Lmax` is the maximum subdiagonal element in the columns of L. This will not exceed the value of the optional parameter **options.lu_factor_tol** (default value $= 5.0$ or 100.0).

`Bmax` is the maximum nonzero element in B (not printed if B_S is factorized).

`BSmax` is the maximum nonzero element in B_S (not printed if B is factorized).

`Umax` is the maximum nonzero element in U, excluding elements of B that remain in U unchanged. (For example, if a slack variable is in the basis, the corresponding row of B will become a row of U without modification. Elements in such rows will not contribute to `Umax`. If the basis is strictly triangular, *none* of the elements of B will contribute, and `Umax` will be zero.)

Ideally, `Umax` should not be significantly larger than `Bmax`. If it is several orders of magnitude larger, it may be advisable to reset the **options.lu_factor_tol** to some value nearer unity.

`Umax` is not printed if B_S is factorized.

`Umin` is the magnitude of the smallest diagonal element of PUQ.

`Growth` is the value of the ratio `Umax`/`Bmax`, which should not be too large.

Providing `Lmax` is not large (say < 10.0), the ratio $\max(\texttt{Bmax}, \texttt{Umax})/\texttt{Umin}$ is an estimate of the condition number of B. If this number is extremely large, the basis is nearly singular and some numerical difficulties might occur. (However, an effort is made to avoid near-singularity by using slacks to replace columns of B that would have made `Umin` extremely small, and the modified basis is refactorized.)

`Lt` is the number of triangular columns of B at the left of L.

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

`d2` is the number of columns remaining when the density of the basis matrix being factorized has reached 0.6.

When **options.print_level** = Nag_Soln_Iter_Full, and **options.crash** $\neq$ Nag_NoCrash (default value **options.crash** = Nag_NoCrash or Nag_CrashThreeTimes), the following lines of intermediate printout are sent to **options.outfile** whenever **options.start** = Nag_Cold. They refer to the number of columns selected by the Crash procedure during each of several passes through A while searching for a triangular basis matrix.

`Slacks` is the number of slacks selected initially.

`Free cols` is the number of free columns in the basis, including those whose bounds are rather far apart.

`Preferred` is the number of 'preferred' columns in the basis (i.e., **options.state**$[j-1] = 3$ for some $j \leq n$). It will be a subset of the columns for which **options.state**$[j-1] = 3$ was specified.

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

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

`Triangle` is the number of triangular columns in the basis with three (or more) nonzeros.

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

When **options.print_level** = Nag_Soln or Nag_Soln_Iter, and **options.print_80ch** = Nag_FALSE, the following lines of final printout (≤ 120 characters) are sent to **options.outfile**.

Let x_j denote the jth 'column variable', for $j = 1, 2, \ldots, n$. We assume that a typical variable x_j has bounds $\alpha \leq x_j \leq \beta$.

The following describes the printout for each column (or variable).

`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` gives the state of x_j relative to the bounds α and β. The various possible states 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` to give some additional information about the state of x_j. Note that unless the optional parameter **options.scale_opt** $= 0$ (default value $= 1$ or 2) is specified, the tests for assigning a key are applied to the variables of the scaled problem.

- `A` *Alternative optimum possible*. x_j is nonbasic, but its reduced gradient is essentially zero. This means that if x_j were allowed to start moving away from its current value, there would be no change in the value of the objective function. The values of the basic and superbasic variables *might* change, giving a genuine alternative solution. The values of the Lagrange multipliers *might* also change.
- `D` *Degenerate*. x_j is basic, but it is equal to (or very close to) one of its bounds.
- `I` *Infeasible*. x_j is basic and is currently violating one of its bounds by more than the value of the optional parameter **options.minor_feas_tol** (default value $= \sqrt{\epsilon}$).
- `N` *Not precisely optimal*. x_j is nonbasic. Its reduced gradient is larger than the value of the optional parameter **options.major_feas_tol** (default value $= \sqrt{\epsilon}$).

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

`Obj Gradient` is the value of g_j at the final iterate. (If any x_j is infeasible, g_j is the gradient of the sum of infeasibilities.)

`Lower Limit` is α, the lower bound specified for x_j. `None` indicates that **bl**$[j-1] \leq -$**options.inf_bound**.

`Upper Limit` is β, the upper bound specified for x_j. `None` indicates that **bu**$[j-1] \geq$ **options.inf_bound**.

`Reduced Gradnt` is the value of d_j at the final iterate.

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

General linear constraints take the form $l \leq Ax \leq u$. Let a_i^{T} denote the ith row of A, for $i = 1, 2, \ldots, n$. The ith constraint is therefore of the form $\alpha \leq a_i^{\mathrm{T}} x \leq \beta$, and the value of $a_i^{\mathrm{T}} x$ is called the *row activity*. Internally, the linear constraints take the form $Ax - s = 0$, where the slack variables s should satisfy

the bounds $l \leq s \leq u$. For the ith 'row', it is the slack variable s_i that is directly available, and it is sometimes convenient to refer to its state. Slacks may be basic or nonbasic (but not superbasic).

Nonlinear constraints $\alpha \leq F_i(x) + a_i^{\mathrm{T}}x \leq \beta$ are treated similarly, except that the row activity and degree of infeasibility are computed directly from $F_i(x) + a_i^{\mathrm{T}}x$ rather than from s_i.

The following describes the printout for each row (or constraint).

`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` gives the state of the ith row relative to the bounds α and β. The various possible states 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 ($\alpha = \beta$).
- `BS` The constraint is not binding. s_i is basic.

A key is sometimes printed before `State` to give some additional information about the state of s_i. Note that unless the optional parameter **options.scale_opt** $= 0$ (default value $= 1$ or 2) is specified, the tests for assigning a key are applied to the variables of the scaled problem.

- `A` *Alternative optimum possible*. s_i is nonbasic, but its reduced gradient is essentially zero. This means that if s_i were allowed to start moving away from its current value, there would be no change in the value of the objective function. The values of the basic and superbasic variables *might* change, giving a genuine alternative solution. The values of the dual variables (or Lagrange multipliers) *might* also change.
- `D` *Degenerate*. s_i is basic, but it is equal to (or very close to) one of its bounds.
- `I` *Infeasible*. s_i is basic and is currently violating one of its bounds by more than the value of the optional parameter **options.minor_feas_tol** (default value $= \sqrt{\epsilon}$).
- `N` *Not precisely optimal*. s_i is nonbasic. Its reduced gradient is larger than the value of the optional parameter **options.major_feas_tol** (default value $= \sqrt{\epsilon}$).

`Activity` is the value of a_i^{Tx} (or $F_i(x) + a_i^{\mathrm{T}}x$ 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 specified for the ith row. `None` indicates that **bl**$[n + i - 1] \leq -$**options.inf_bound**.

`Upper Limit` is β, the upper bound specified for the ith row. `None` indicates that **bu**$[n + i - 1] \geq$ **options.inf_bound**.

`Dual Activity` is the value of the dual variable π_i.

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

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