

## 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, Nag_Error *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:

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

where  $x = (x_1, x_2, \dots, x_n)^T$  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  $j$ th 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 argument **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  $s = (s_1, s_2, \dots, s_m)^T$ . 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:

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

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  $(B | N)$ , 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 argument **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

$$f(x') + c^T x' + d^T y',$$

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 **njnl** (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

$$\begin{pmatrix} F(x'') & A_2 y'' \\ A_3 x'' & A_4 y'' \end{pmatrix}, \quad (3)$$

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

The inequalities  $l_1 \leq F(x'') + A_2 y'' \leq u_1$  and  $l_2 \leq A_3 x'' + A_4 y'' \leq u_2$  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**  $\leq$  **njnl** (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**  $>$  **njnl** and  $x' = (x'', x''')$ , where the objective is nonlinear in just the last vector  $x'''$ . The first **njnl** 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  $\epsilon$  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 ( $= \frac{\partial F}{\partial x}$ ) for a specified **njnl** ( $\leq n$ ) element vector  $x$ . If there are no nonlinear constraints (i.e., **ncnl** = 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 njnl, Integer nnzjac,
             const double x[], double conf[], double conjac[],
             Nag_Comm *comm)
```

- 1: **ncnl** – Integer *Input*
- On entry:* the number of nonlinear constraints. These must be the first **ncnl** constraints in the problem.
- 2: **njnl** – Integer *Input*
- On entry:* the number of nonlinear variables. These must be the first **njnl** variables in the problem.

3:	<b>nnzjac</b> – Integer	<i>Input</i>
	<i>On entry:</i> the number of nonzero elements in the constraint Jacobian. Note that <b>nnzjac</b> will always be less than, or equal to, <b>ncnln</b> × <b>njnl</b> .	
4:	<b>x[njnl]</b> – const double	<i>Input</i>
	<i>On entry:</i> $x$ , 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:	<b>conf[ncnln]</b> – double	<i>Output</i>
	<i>On exit:</i> if <b>comm</b> → <b>flag</b> = 0 or 2, <b>conf</b> [ $i - 1$ ] must contain the value of $F_i(x)$ , the $i$ th nonlinear constraint at $x$ .	
6:	<b>conjac[nnzjac]</b> – double	<i>Output</i>
	<i>On exit:</i> if <b>comm</b> → <b>flag</b> = 1 or 2, <b>conjac</b> must return the available elements of $J(x)$ , the constraint Jacobian evaluated at $x$ . These elements must be stored in <b>conjac</b> in exactly the same positions as implied by the definitions of the arrays <b>a</b> , <b>ha</b> and <b>ka</b> 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 argument <b>options.verify_grad</b> ), so great care is essential.	
	If all elements of the constraint Jacobian are known, i.e., the optional argument <b>options.con_deriv</b> = Nag_TRUE (the default), any constant elements of the Jacobian may be assigned to <b>a</b> at the start of the optimization if desired. If an element of <b>conjac</b> is not assigned in <b>confun</b> , the corresponding value from <b>a</b> is used. See also the description for <b>a</b> .	
	If <b>options.con_deriv</b> = Nag_FALSE, then any available partial derivatives of $c_i(x)$ must be assigned to the elements of <b>conjac</b> ; the remaining elements <i>must remain unchanged</i> . It must be emphasized that, in that case, unassigned elements of <b>conjac</b> are not treated as constant; they are estimated by finite differences, at non-trivial expense.	
7:	<b>comm</b> – Nag_Comm *	
	Pointer to a structure of type Nag_Comm; the following members are relevant to <b>confun</b> .	
	<b>flag</b> – Integer	<i>Input/Output</i>
	<i>On entry:</i> <b>confun</b> is called with <b>comm</b> → <b>flag</b> set to 0, 1 or 2.	
	If <b>comm</b> → <b>flag</b> = 0, only <b>conf</b> has to be referenced.	
	If <b>comm</b> → <b>flag</b> = 1, only <b>conjac</b> has to be referenced.	
	If <b>comm</b> → <b>flag</b> = 2, both <b>conf</b> and <b>conjac</b> are referenced.	
	<i>On exit:</i> if <b>confun</b> resets <b>comm</b> → <b>flag</b> 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 <b>confun</b> resets <b>comm</b> → <b>flag</b> 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 <b>fail</b> is supplied to nag_opt_nlp_sparse (e04ugc), <b>fail.errnum</b> will be set to your setting of <b>comm</b> → <b>flag</b> .	
	<b>first</b> – Nag_Boolean	<i>Input</i>
	<i>On entry:</i> will be set to Nag_TRUE on the first call to <b>confun</b> 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 arguments **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 argument **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 ( $= \frac{\partial f}{\partial x}$ ) for a specified **nonln** ( $\leq n$ ) 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  $\frac{\partial f}{\partial x}$  evaluated at the current point  $x$ .

If the optional argument **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 arguments **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 argument **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:*  $n \geq 1$ .

- 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:*  $m \geq 1$ .
- 5: **ncnln** – Integer *Input*  
*On entry:* the number of nonlinear constraints. These correspond to the leading **ncnln** rows of  $A$ .  
*Constraint:*  $0 \leq \text{ncnln} \leq m$ .
- 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 **njnl**.)  
*Constraint:*  $0 \leq \text{nonln} \leq n$ .
- 7: **njnl** – Integer *Input*  
*On entry:* the number of nonlinear Jacobian variables. If there are any nonlinear constraints, the leading **njnl** columns of  $A$  belong to the nonlinear Jacobian variables. If **nonln**  $>$  0 and **njnl**  $>$  0, the nonlinear objective and Jacobian variables overlap. The total number of nonlinear variables is given by  $\bar{n} = \max(\text{nonln}, \text{njnl})$ .  
*Constraints:*  
if **ncnln** = 0, **njnl** = 0;  
if **ncnln**  $>$  0,  $1 \leq \text{njnl} \leq n$ .
- 8: **iobj** – Integer *Input*  
*On entry:* if **iobj**  $>$  **ncnln**, row **iobj** of  $A$  is a free row containing the nonzero elements of the linear part of the objective function.  
**iobj** = 0  
There is no free row.  
**iobj** = -1  
There is a dummy ‘free’ row.  
*Constraints:*  
if **iobj**  $>$  0, **ncnln**  $<$  **iobj**  $\leq m$ ;  
otherwise **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 **iobj** = -1, set **nnz** = 1.  
*Constraint:*  $1 \leq \text{nnz} \leq n \times m$ .
- 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 argument `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  $\mathbf{a}$ . 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  $|\beta| < \text{bigbnd}$  and `bigbnd` is the value of the optional argument `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  $i = 1, 2, \dots, \text{nnz}$ . 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:*  $1 \leq \text{ha}[i - 1] \leq \mathbf{m}$ , for  $i = 1, 2, \dots, \text{nnz}$ .

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

*On entry:* `ka[j - 1]` must contain the index in  $\mathbf{a}$  of the start of the  $j$ th column, for  $j = 1, 2, \dots, \mathbf{n}$ . To specify the  $j$ th 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  $j = 1, 2, \dots, \mathbf{n}$ .

*Constraints:*

$$\begin{aligned} \mathbf{ka}[0] &= 0; \\ \mathbf{ka}[j - 1] &\geq 0, \text{ for } j = 2, 3, \dots, \mathbf{n}; \\ \mathbf{ka}[\mathbf{n}] &= \text{nnz}; \\ 0 \leq \mathbf{ka}[j] - \mathbf{ka}[j - 1] &\leq \mathbf{m}, \text{ for } j = 1, 2, \dots, \mathbf{n}. \end{aligned}$$

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  $\mathbf{n}$  elements of `bl` must contain the bounds on the variables  $\mathbf{x}$ , the next `ncnl` elements the bounds for the nonlinear constraints  $F(x)$  (if any) and the next  $(\mathbf{m} - \text{ncnl})$  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] ≤ -options.inf_bound`, and to specify a nonexistent upper bound (i.e.,  $u_j = +\infty$ ), set `bu[j - 1] ≥ options.inf_bound`, where `options.inf_bound` is one of the optional arguments (default value  $10^{20}$ , see Section 12.2). To specify the  $j$ th constraint as an *equality*, set `bl[j - 1] = bu[j - 1] =  $\beta$` , say, where  $|\beta| < \text{options.inf_bound}$ . Note that the lower bound corresponding to `iobj ≠ 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:*

$$\begin{aligned} \mathbf{bl}[j] &\leq \mathbf{bu}[j], \text{ for } j = 0, 1, \dots, \mathbf{n} + \mathbf{m} - 1; \\ \text{if } \mathbf{bl}[j] = \mathbf{bu}[j] = \beta, &|\beta| < \text{options.inf_bound}; \\ \text{if } \text{ncnl} < \text{iobj} \leq \mathbf{m} &\text{ or } \text{iobj} = -1, \mathbf{bl}[\mathbf{n} + |\text{iobj}| - 1] \leq -\text{options.inf_bound} \text{ and} \\ \mathbf{bu}[\mathbf{n} + |\text{iobj}| - 1] &\geq \text{options.inf_bound}. \end{aligned}$$

- 15: **xs**[**n** + **m**] – double *Input/Output*  
*On entry:* **xs**[ $j - 1$ ], for  $j = 1, 2, \dots, \mathbf{n}$ , must contain the initial values of the variables,  $x$ . In addition, if a ‘warm start’ is specified by means of the optional argument **options.start** (see Section 12.2) the elements **xs**[ $\mathbf{n} + i - 1$ ], for  $i = 1, 2, \dots, \mathbf{m}$ , 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 argument **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 argument **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 3.2.1.1 in the Essential Introduction).  
*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 arguments 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 argument **options.start** in Section 12.2).  
 If any of these optional arguments are required then the structure **options** should be declared and initialized by a call to `nag_opt_init` (e04xxc) and supplied as an argument to `nag_opt_nlp_sparse` (e04ugc). However, if the optional arguments 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 3.6 in the Essential Introduction).

## 5.1 Description of Printed Output

Intermediate and final results are printed out by default. The level of printed output can be controlled with the structure 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 ( $\leq 80$  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 arguments (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 argument <b>options.elastic_wt</b> (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 <i>rowerr</i> , the largest element of the scaled nonlinear constraint residual vector defined in the description of the optional argument <b>options.major_feas_tol</b> . The solution is regarded as ‘feasible’ if Feasibl is less than (or equal to) the <b>options.major_feas_tol</b> (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 <i>maxgap</i> , the largest element of the maximum complementarity gap vector defined in the description of the optional argument <b>options.major_opt_tol</b> . The Lagrange multipliers are regarded as ‘optimal’ if Optimal is less than (or equal to) the optional argument <b>options.major_opt_tol</b> (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 <b>ncnl</b> and <b>nonln</b> 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 $R^T R$ 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 arguments <b>options.major_feas_tol</b> and <b>options.major_opt_tol</b> . 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 arguments **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 argument **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 argument **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 argument **options.cnames** = **NULL**, a default name is assigned to the  $j$ th variable, for  $j = 1, 2, \dots, n$ . Otherwise, the name supplied in **options.cnames**[ $j - 1$ ] is assigned to the  $j$ th 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 argument `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 argument `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 argument `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 $\mathbf{bl}[j-1] \leq -\mathbf{options.inf\_bound}$ .
Upper Bound	is the upper bound specified for the variable. None indicates that $\mathbf{bu}[j-1] \geq \mathbf{options.inf\_bound}$ .
Lagr Mult	is the Lagrange multiplier for the associated bound. This will be zero if <code>State</code> is FR. If $x$ is optimal, the multiplier should be non-negative if <code>State</code> is LL, non-positive if <code>State</code> is UL, and zero if <code>State</code> is BS or SBS.
Residual	is the difference between the variable <code>Value</code> and the nearer of its (finite) bounds $\mathbf{bl}[j-1]$ and $\mathbf{bu}[j-1]$ . A blank entry indicates that the associated variable is not bounded (i.e., $\mathbf{bl}[j-1] \leq -\mathbf{options.inf\_bound}$ and $\mathbf{bu}[j-1] \geq \mathbf{options.inf\_bound}$ ).

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.cnames[j-1]` replaced by `options.cnames[n+j-1]`,  $\mathbf{bl}[j-1]$  and  $\mathbf{bu}[j-1]$  replaced by  $\mathbf{bl}[n+j-1]$  and  $\mathbf{bu}[n+j-1]$  respectively, and with the following 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, `njnl` =  $\langle value \rangle$  while `ncnl` =  $\langle value \rangle$ . These arguments must satisfy `njnl` = 0 when `ncnl` = 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, **ncnl** =  $\langle value \rangle$ , **iobj** =  $\langle value \rangle$  and **m** =  $\langle value \rangle$ . These arguments must satisfy **ncnl** < **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: **ka**[0] = 0.

The contents of array **ka** are not valid.  
Constraint: **ka**[**n**] = **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 argument **options.lu\_factor\_tol** (default value = 5.0 or 100.0) is too large.

### NE\_BOUND

The lower bound for variable  $\langle value \rangle$  (array element **bl**[ $\langle value \rangle$ ]) is greater than the upper bound.

### NE\_BOUND\_EQ

The lower bound and upper bound for variable  $\langle value \rangle$  (array elements **bl**[ $\langle value \rangle$ ] and **bu**[ $\langle value \rangle$ ]) 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  $\langle value \rangle$  (array element **bl**[ $\langle value \rangle$ ] and **bu**[ $\langle value \rangle$ ]) 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  $\langle value \rangle$  (array element **bl**[ $\langle value \rangle$ ] and **bu**[ $\langle value \rangle$ ]) are equal but they are greater than or equal to **options.inf\_bound**.

**NE\_BOUND\_LCON**

The lower bound for linear constraint  $\langle value \rangle$  (array element **bl**[ $\langle value \rangle$ ]) is greater than the upper bound.

**NE\_BOUND\_NLCON**

The lower bound for nonlinear constraint  $\langle value \rangle$  (array element **bl**[ $\langle value \rangle$ ]) 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  $\langle value \rangle$ , column  $\langle value \rangle$ .

**NE\_INT\_ARG\_LT**

On entry, **iobj** =  $\langle value \rangle$ .

Constraint: **iobj**  $\geq -1$ .

On entry, **m** =  $\langle value \rangle$ .

Constraint: **m**  $\geq 1$ .

On entry, **n** =  $\langle value \rangle$ .

Constraint: **n**  $\geq 1$ .

**NE\_INT\_ARRAY\_1**

Value  $\langle value \rangle$  given to **ka**[ $\langle value \rangle$ ] not valid. Correct range for elements of **ka** is  $\geq 0$ .

**NE\_INT\_ARRAY\_2**

Value  $\langle value \rangle$  given to **ha**[ $\langle value \rangle$ ] is not valid. Correct range for elements of **ha** is 1 to **m**.

**NE\_INT\_OPT\_ARG\_GT**

On entry, **options.con\_check\_start** =  $\langle value \rangle$ .

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** =  $\langle value \rangle$ .

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** =  $\langle value \rangle$ .

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** =  $\langle value \rangle$ .

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** =  $\langle value \rangle$ .

Constraint: **options.con\_check\_start**  $\geq 1$ .

(Note that this error may only occur when **options.verify\_grad** = Nag\_CheckCon or Nag\_CheckObjCon.)

On entry, **options.con\_check\_stop** =  $\langle value \rangle$ .

Constraint: **options.con\_check\_stop**  $\geq 1$ .

(Note that this error may only occur when **options.verify\_grad** = Nag\_CheckCon or Nag\_CheckObjCon.)

On entry, **options.expand\_freq** =  $\langle value \rangle$ .

Constraint: **options.expand\_freq**  $\geq 0$ .

On entry, **options.factor\_freq** =  $\langle value \rangle$ .

Constraint: **options.factor\_freq**  $\geq 0$ .

On entry, **options.fcheck** =  $\langle value \rangle$ .

Constraint: **options.fcheck**  $\geq 0$ .

On entry, **options.obj\_check\_start** =  $\langle value \rangle$ .

Constraint: **options.obj\_check\_start**  $\geq 1$ .

(Note that this error may only occur when **options.verify\_grad** = Nag\_CheckObj or Nag\_CheckObjCon.)

On entry, **options.obj\_check\_stop** =  $\langle value \rangle$ .

Constraint: **options.obj\_check\_stop**  $\geq 1$ .

(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  $\langle value \rangle$  given to **ncnl** is not valid. Correct range is 0 to **m**.

Value  $\langle value \rangle$  given to **njnl** is not valid. Correct range is (when **ncnl** > 0) 1 to **n**.

Value  $\langle value \rangle$  given to **nnz** is not valid. Correct range is 1 to **n**  $\times$  **m**.

Value  $\langle value \rangle$  given to **nonln** is not valid. Correct range is 0 to **n**.

Value  $\langle value \rangle$  given to **options.hess\_freq** is not valid. Correct range is **options.hess\_freq** > 0.

Value  $\langle value \rangle$  given to **options.hess\_update** is not valid. Correct range is **options.hess\_update**  $\geq 0$ .

Value  $\langle value \rangle$  given to **options.iter\_lim** is not valid. Correct range is **options.iter\_lim** > 0.

Value  $\langle value \rangle$  given to **options.major\_iter\_lim** is not valid. Correct range is **options.major\_iter\_lim**  $\geq 0$ .

Value  $\langle value \rangle$  given to **options.max\_sb** is not valid. Correct range is **options.max\_sb** > 0.

Value  $\langle value \rangle$  given to **options.minor\_iter\_lim** is not valid. Correct range is **options.minor\_iter\_lim**  $\geq 0$ .

Value  $\langle value \rangle$  given to **options.nsb** is not valid. Correct range is: if **options.start** = Nag\_Warm, then **options.nsb**  $\geq 0$ .

Value  $\langle value \rangle$  given to **options.part\_price** is not valid. Correct range is **options.part\_price** > 0.

**NE\_INVALID\_INT\_RANGE\_2**

Value  $\langle value \rangle$  given to **options.scale\_opt** is not valid. Correct range is  $0 \leq \mathbf{options.scale\_opt} \leq 2$ .



**NE\_INVALID\_REAL\_RANGE\_E**

Value  $\langle value \rangle$  given to **options.elastic\_wt** is not valid. Correct range is **options.elastic\_wt**  $> 0.0$ .

Value  $\langle value \rangle$  given to **options.inf\_bound** is not valid. Correct range is **options.inf\_bound**  $> 0.0$ .

Value  $\langle value \rangle$  given to **options.inf\_step** is not valid. Correct range is **options.inf\_step**  $> 0.0$ .

Value  $\langle value \rangle$  given to **options.lu\_den\_tol** is not valid. Correct range is **options.lu\_den\_tol**  $\geq 0.0$ .

Value  $\langle value \rangle$  given to **options.lu\_factor\_tol** is not valid. Correct range is **options.lu\_factor\_tol**  $\geq 1.0$ .

Value  $\langle value \rangle$  given to **options.lu\_sing\_tol** is not valid. Correct range is **options.lu\_sing\_tol**  $> 0.0$ .

Value  $\langle value \rangle$  given to **options.lu\_update\_tol** is not valid. Correct range is **options.lu\_update\_tol**  $\geq 1.0$ .

Value  $\langle value \rangle$  given to **options.major\_feas\_tol** is not valid. Correct range is **options.major\_feas\_tol**  $> \epsilon$ .

Value  $\langle value \rangle$  given to **options.major\_opt\_tol** is not valid. Correct range is **options.major\_opt\_tol**  $> 0.0$ .

Value  $\langle value \rangle$  given to **options.major\_step\_lim** is not valid. Correct range is **options.major\_step\_lim**  $> 0.0$ .

Value  $\langle value \rangle$  given to **options.minor\_feas\_tol** is not valid. Correct range is **options.minor\_feas\_tol**  $> \epsilon$ .

Value  $\langle value \rangle$  given to **options.minor\_opt\_tol** is not valid. Correct range is **options.minor\_opt\_tol**  $> 0.0$ .

Value  $\langle value \rangle$  given to **options.nz\_coef** is not valid. Correct range is **options.nz\_coef**  $\geq 1.0$ .

Value  $\langle value \rangle$  given to **options.pivot\_tol** is not valid. Correct range is **options.pivot\_tol**  $> 0.0$ .

Value  $\langle value \rangle$  given to **options.unbounded\_obj** is not valid. Correct range is **options.unbounded\_obj**  $> 0.0$ .

Value  $\langle value \rangle$  given to **options.violation\_limit** is not valid. Correct range is **options.violation\_limit**  $> 0.0$ .

**NE\_INVALID\_REAL\_RANGE\_EE**

Value  $\langle value \rangle$  given to **options.c\_diff\_int** is not valid. Correct range is  $\epsilon \leq$  **options.c\_diff\_int**  $< 1.0$ .

Value  $\langle value \rangle$  given to **options.crash\_tol** is not valid. Correct range is  $0.0 \leq$  **options.crash\_tol**  $< 1.0$ .

Value  $\langle value \rangle$  given to **options.f\_diff\_int** is not valid. Correct range is  $\epsilon \leq$  **options.f\_diff\_int**  $< 1.0$ .

Value  $\langle value \rangle$  given to **options.f\_prec** is not valid. Correct range is  $\epsilon \leq$  **options.f\_prec**  $< 1.0$ .

Value  $\langle value \rangle$  given to **options.linesearch\_tol** is not valid. Correct range is  $0.0 \leq$  **options.linesearch\_tol**  $< 1.0$ .

Value  $\langle value \rangle$  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:  $\langle value \rangle$ .

The problem is infeasible. The linear constraints cannot all be satisfied to within the values of the optional argument **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 arguments **options.unbounded\_obj** (default value =  $10^{15}$ ) and **options.inf\_step** (default value =  $\max(\text{bigbnd}, 10^{20})$ ) 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 argument **options.violation\_limit** (default value = 10.0).

**NE\_NAME\_TOO\_LONG**

The string pointed to by **options.cnames**[*value*] 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 arguments **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: *value*.

The problem is infeasible. The nonlinear constraints cannot all be satisfied to within the values of the optional argument **options.major\_feas\_tol** (default value =  $\sqrt{\epsilon}$ ).

**NE\_NOT\_APPEND\_FILE**

Cannot open file *string* for appending.

**NE\_NOT\_CLOSE\_FILE**

Cannot close file *string*.

**NE\_NOT\_REQUIRED\_ACC**

Feasible solution, but required accuracy could not be achieved.

Check that the value of the optional argument **options.major\_opt\_tol** (default value =  $\sqrt{\epsilon}$ ) is not too small.

**NE\_OBJ\_BOUND**

Invalid lower bound for objective row. Bound should be  $\leq -\text{options.inf\_bound}$ .

Invalid upper bound for objective row. Bound should be  $\geq \text{options.inf\_bound}$ .

**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**[ $\langle value \rangle$ ] is out of range. **options.state**[ $\langle value \rangle$ ] =  $\langle value \rangle$ .

**NE\_SUPERBASICS\_LIMIT**

Too many superbasic variables (**options.max\_sb** =  $\langle value \rangle$ ).

The value of the optional argument **options.max\_sb** (default value =  $\min(500, \bar{n} + 1, n)$ ) is too small and should be increased.

**NE\_TOO\_MANY\_ITER**

Iteration limit (**options.iter\_lim** =  $\langle value \rangle$ ) exceeded.

**NE\_TOO\_MANY\_MAJOR\_ITER**

Major iteration limit (**options.major\_iter\_lim** =  $\langle value \rangle$ ) exceeded.

**NE\_TOO\_MANY\_MINOR\_ITER**

Minor iteration limit (**options.minor\_iter\_lim** =  $\langle value \rangle$ ) 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 =  $\langle value \rangle$ .

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 approximately  $d$  correct digits.

**8 Parallelism and Performance**

Not applicable.

**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 arguments **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

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

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

$$x_0 = (0, 0, 0, 0)^T,$$

and  $f(x_0) = 0$ .

The optimal solution (to five figures) is

$$x^* = (0.11887, -0.39623, 679.94, 1026.0)^T,$$

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 **njnl** = 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 **njnl** = 4 nonlinear constraint variables, but, as mentioned earlier, it is preferable to keep the size of the nonlinear Jacobian ( $J$ ) small, having **nonln** > **njnl**.)

The Jacobian matrix  $A$  is the  $\mathbf{m} = 6$  by  $\mathbf{n} = 4$  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 **ncnl** = 3 nonlinear constraints, rows 4 and 5 define the 2 linear constraints and there is finally an **iobj** = 6th 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  $1.0e + 25$ ). Effective Jacobian values will be provided in the argument **conjac**[ $i - 1$ ], for  $i = 1, 2, \dots, \mathbf{nnzjac}$ , **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  $\mathbf{bl} = (-0.55, -0.55, 0.0, 0.0, -894.6, -894.6, -1294.8, -0.55, -0.55, -1.0e + 25)^T$ , and  $\mathbf{bu} = (0.55, 0.55, 1200.0, 1200.0, -894.6, -894.6, -1294.8, 1.0e + 25, 1.0e + 25, 1.0e + 25)^T$ .

The first  $n = 4$  elements of  $\mathbf{bl}$  and  $\mathbf{bu}$  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 arguments 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.
 *
 * Copyright 2000 Numerical Algorithms Group.
 *
 * NAG C Library
 *
 * Mark 6, 2000.
 * Mark 7 revised, 2001.
 * Mark 8 revised, 2004.
 */

#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]
#define MAXNAMES 300

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;
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*/
scanf(" %*[\n]");
/* Read the problem dimensions */
scanf(" %*[\n]");
scanf("%ld%ld", &n, &m);
/* Read NCNLN, NONLN and NJNLN from data file. */
scanf(" %*[\n]");
scanf("%ld%ld%ld", &ncnl, &nonln, &njnl);
/* Read NNZ, IOBJ */
scanf(" %*[\n]");
scanf("%ld%ld", &nnz, &iobj);

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 */
scanf(" %*[\n]");
scanf(" %*['']");
for (i = 0; i < n+m; ++i)
{
    scanf(" '%8c'", &NAMES(i, 0));
    NAMES(i, 8) = '\0';
    crnames[i] = &NAMES(i, 0);
}

/* read the matrix and set up ka. */
jcol = 1;
ka[jcol - 1] = 0;
scanf(" %*[\n]");
for (i = 0; i < nnz; ++i)
{
    /* a[i] stores (ha[i], icol) element of matrix */
    scanf("%lf%ld%ld", &a[i], &ha[i], &icol);
    if (icol < jcol)
    {
        /* Elements not ordered by increasing column index. */
        printf("Element in column%5ld found after element in"
              " column%5ld. 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 */
scanf("%i^\n");
for (i = 0; i < n + m; ++i)
    scanf("%lf", &bl[i]);
scanf("%i^\n");
for (i = 0; i < n + m; ++i)
    scanf("%lf", &bu[i]);

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

/* Initialize the options structure */
/* nag_opt_init (e04xxc).
 * Initialization function for option setting
 */
nag_opt_init(&options);
/* 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) Nag_TRUE,
            "stdout", &fail);
/* Set some other options directly */
options.major_iter_lim = 100;
options.cnames = cnames;

/* 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;
}

/* We perturb the solution and solve the
 * same problem again using a warm start.
 */
printf("\n\n\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;
options.print_level = Nag_Iter;

/* 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, njln, 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;
}
/* 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 njln, 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

Optional parameter setting for e04ugc.

-----  
Option file: e04ugce.opt

```
minor_iter_lim = 20
iter_lim = 30
```

Parameters to e04ugc

```
-----
Frequencies.
fcheck..... 60          expand_freq..... 10000
factor_freq..... 50

QP subproblems.
scale_tol..... 9.00e-01  minor_feas_tol..... 1.05e-08
scale_opt..... 1          minor_opt_tol..... 1.05e-08
part_price..... 1          crash_tol..... 1.00e-01
pivot_tol..... 2.04e-11  minor_print_level.... Nag_NoPrint
crash..... Nag_NoCrash  elastic_wt..... 1.00e+02

Derivatives.
obj_deriv..... Nag_TRUE   con_deriv..... Nag_TRUE
verify_grad..... Nag_SimpleCheck  print_deriv..... Nag_D_Print
Start obj check at col.. 1      Stop obj check at col.. 4
Start con check at col.. 1      Stop con check at col.. 2

The SQP method.
direction..... Nag_Minimize
Nonlinear objective vars 4      major_opt_tol..... 1.05e-08
f_prec..... 1.72e-13  inf_step..... 1.00e+20
max_sb..... 4          f_diff_int..... 4.15e-07
unbounded_obj..... 1.00e+15  c_diff_int..... 5.56e-05
major_step_lim..... 2.00e+00  deriv_linesearch..... Nag_TRUE
print_level..... Nag_Soln_Iter  major_iter_lim..... 100
linesearch_tol..... 9.00e-01  minor_iter_lim..... 20
inf_bound..... 1.00e+20  iter_lim..... 30

Hessian approximation.
hess_storage..... Nag_HessianFull  hess_update..... 20
hess_freq..... 99999999

Nonlinear constraints.
Nonlinear constraints... 3      major_feas_tol..... 1.05e-08
Nonlinear Jacobian vars. 2      violation_limit..... 1.00e+01

Miscellaneous.
Variables..... 4          Linear constraints..... 3
Nonlinear variables..... 4      Linear variables..... 0
lu_factor_tol..... 5.00e+00  lu_sing_tol..... 2.04e-11
lu_update_tol..... 5.00e+00  lu_den_tol..... 6.00e-01
eps (machine precision). 1.11e-16
start..... Nag_Cold      feas_exit..... Nag_FALSE
Names..... supplied      print_80ch..... Nag_TRUE
outfile..... stdout

Memory allocation.
nz_coef..... 5.00e+00  Initial sizes of work arrays.
```

```
state..... Nag      Integers..... 1628
lambda..... Nag      Reals..... 1258
```

```
XXX Scale option reduced from      1 to      0.
XXX Feasible linear rows.
XXX Norm(x-x0) minimized. Sum of infeasibilities = 0.00e+00.
```

```
confun sets      6 out of      6 constraint gradients.
objfun sets      4 out of      4 objective gradients.
```

-----  
Verification of constraint gradients returned by subroutine confun  
-----

Cheap test on confun...

The Jacobian seems to be OK.

The largest discrepancy was 4.41e-08 in constraint 2.

-----  
Verification of objective gradients returned by subroutine objfun  
-----

Cheap test on objfun...

The objective gradients seem to be OK.

```
Gradient projected in two directions 0.00000000000e+00 0.00000000000e+00
Difference approximations           1.74111992322e-19 4.48742248252e-21
```

XXX All-slack basis B = I selected.

XXX Large multipliers.

Elastic mode started with weight = 2.0e+02.

Maj	Mnr	Step	Merit Function	Feasibl	Optimal	Cond Hz PD			
0	8	0.0e+00	3.199952e+05	1.7e+00	8.0e-01	1.0e+00	FF	R	i
1	4	1.0e+00	2.419951e+05	7.7e-01	3.7e+01	1.0e+00	FF	s	
2	1	1.0e+00	5.172188e+03	2.9e-02	1.9e+00	1.0e+00	FF		
3	1	3.8e-01	5.038588e+03	1.8e-02	4.6e+00	1.2e+02	FF		
4	1	3.6e-01	5.120830e+03	1.2e-02	2.0e+00	1.6e+02	FF		
5	1	1.0e+00	5.126491e+03	1.0e-04	3.6e-02	1.7e+02	FF		
6	1	3.1e-01	5.126498e+03	7.1e-05	3.1e-02	1.1e+02	FF		
7	1	1.0e+00	5.126498e+03	4.3e-09	6.5e-04	1.1e+02	TF		
8	1	1.0e+00	5.126498e+03	4.5e-13	4.8e-05	1.1e+02	TF		
9	0	1.0e+00	5.126498e+03	1.2e-15	3.5e-13	1.1e+02	TT		

Exit from NP problem after 9 major iterations,  
19 minor iterations.

Variable	State	Value	Lower Bound	Upper Bound	Lagr Mult	Residual
Varble 1	BS	1.188764e-01	-5.50000e-01	5.50000e-01	-1.8190e-12	4.3112e-01
Varble 2	BS	-3.962336e-01	-5.50000e-01	5.50000e-01	1.6371e-11	1.5377e-01
Varble 3	BS	6.799453e+02	0.00000e+00	1.20000e+03	-2.9310e-14	5.2005e+02
Varble 4	SBS	1.026067e+03	0.00000e+00	1.20000e+03	-6.6613e-14	1.7393e+02

Constrnt	State	Value	Lower Bound	Upper Bound	Lagr Mult	Residual
NlnCon 1	EQ	-8.948000e+02	-8.94800e+02	-8.94800e+02	-4.3870e+00	3.4106e-12
NlnCon 2	EQ	-8.948000e+02	-8.94800e+02	-8.94800e+02	-4.1056e+00	4.5475e-13
NlnCon 3	EQ	-1.294800e+03	-1.29480e+03	-1.29480e+03	-5.4633e+00	3.4106e-12
LinCon 1	BS	2.773572e-01	-5.50000e-0	None 25	0.0000e+00	8.2736e-01
LinCon 2	BS	-2.773572e-01	-5.50000e-0	None 25	0.0000e+00	2.7264e-01

Free Row BS 4.091970e+03 None None 25 -1.0000e+00 4.0920e+03

Exit e04ugc - Optimal solution found.

Final objective value = 5126.498

A run of the same example with a warm start:

-----  
Parameters to e04ugc  
-----

Frequencies.

fcheck.....	60	expand_freq.....	10000
factor_freq.....	50		

QP subproblems.

scale_tol.....	9.00e-01	minor_feas_tol.....	1.05e-08
scale_opt.....	1	minor_opt_tol.....	1.05e-08
part_price.....	1	crash_tol.....	1.00e-01
pivot_tol.....	2.04e-11	minor_print_level.....	Nag_NoPrint
crash.....	Nag_NoCrash	elastic_wt.....	1.00e+02

Derivatives.

obj_deriv.....	Nag_TRUE	con_deriv.....	Nag_TRUE
verify_grad.....	Nag_SimpleCheck	print_deriv.....	Nag_D_NoPrint
Start obj check at col..	1	Stop obj check at col..	4
Start con check at col..	1	Stop con check at col..	2

The SQP method.

direction.....	Nag_Minimize	major_opt_tol.....	1.05e-08
Nonlinear objective vars	4	inf_step.....	1.00e+20
f_prec.....	1.72e-13	f_diff_int.....	4.15e-07
max_sb.....	4	c_diff_int.....	5.56e-05
unbounded_obj.....	1.00e+15	deriv_linesearch.....	Nag_TRUE
major_step_lim.....	2.00e+00	major_iter_lim.....	100
print_level.....	Nag_Iter	minor_iter_lim.....	20
linesearch_tol.....	9.00e-01	iter_lim.....	30
inf_bound.....	1.00e+20		

Hessian approximation.

hess_storage.....	Nag_HessianFull	hess_update.....	20
hess_freq.....	99999999		

Nonlinear constraints.

Nonlinear constraints...	3	major_feas_tol.....	1.05e-08
Nonlinear Jacobian vars.	2	violation_limit.....	1.00e+01

Miscellaneous.

Variables.....	4	Linear constraints.....	3
Nonlinear variables.....	4	Linear variables.....	0
lu_factor_tol.....	5.00e+00	lu_sing_tol.....	2.04e-11
lu_update_tol.....	5.00e+00	lu_den_tol.....	6.00e-01
eps (machine precision).	1.11e-16	feas_exit.....	Nag_FALSE
start.....	Nag_Warm	print_80ch.....	Nag_TRUE
Names.....	supplied		
outfile.....	stdout		

Memory allocation.

nz_coef.....	5.00e+00	Initial sizes of work arrays.	
state.....	Nag	Integers.....	1628
lambda.....	Nag	Reals.....	1258

XXX Scale option reduced from 1 to 0.  
 XXX Feasible linear rows.  
 XXX Norm(x-x0) minimized. Sum of infeasibilities = 0.00e+00.  
 XXX All-slack basis B = I selected.

Maj	Mnr	Step	Merit Function	Feasibl	Optimal	Cond	Hz	PD	
0	1	0.0e+00	5.128197e+03	1.3e-01	1.1e+00	1.7e+00	FF		R
1	1	1.0e+00	4.883655e+03	3.5e-03	5.7e-01	2.0e+02	FF		S
2	1	1.8e-01	5.126320e+03	2.8e-03	3.7e+00	1.9e+02	FF		
3	1	2.8e-01	5.126417e+03	2.0e-03	1.1e+00	1.9e+02	FF		
4	1	1.0e+00	5.126499e+03	3.2e-06	1.9e-01	2.0e+02	FF		
5	1	1.0e+00	5.126498e+03	1.1e-08	4.2e-02	1.1e+02	FF		
6	1	1.0e+00	5.126498e+03	2.2e-09	1.2e-06	1.1e+02	TF		
7	1	1.0e+00	5.126498e+03	4.0e-17	2.7e-10	1.1e+02	TT		

Exit from NP problem after 7 major iterations,  
8 minor iterations.

Exit e04ugc - Optimal solution found.

Final objective value = 5126.498

## 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  $j$ th 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–Karash–Tucker (KKT) point* for (1) (see, e.g., Powell (1974)) if the following conditions hold:

- $x$  is feasible;
- there exists a vector  $\lambda$  (*the Lagrange multiplier vector for the bound and general constraints*) such that

$$g(x) = r'(x)^T \lambda = (I \quad J(x)^T \quad G^T) \lambda, \quad (4)$$

where  $g$  is the gradient of  $f$  evaluated at  $x$ ;

- the Lagrange multiplier  $\lambda_j$  associated with the  $j$ th 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  $\lambda_j$  can have any value if  $l_j = u_j$ .

An equivalent statement of the condition (4) is

$$Z^T g(x) = 0,$$

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

$$N = \left\{ z \mid r'_j(x)z = 0 \quad \text{for all } j \in \mathcal{G} \right\}.$$

The columns of  $Z$  may then be taken as any basis for the vector space  $N$ . The vector  $Z^T g$  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

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

where  $x$  and  $s = (s_N, s_L)^T$  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

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

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*  $\pi_i$ . 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  $g - A^T\pi$ , 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  $\pi$ . 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 argument **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

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

where  $D$  is a diagonal matrix of penalty arguments. If  $(x_k, s_k, \pi_k)$  denotes the current estimate of the solution and  $(\hat{x}, \hat{s}, \hat{\pi})$  denotes the optimal QP solution, the linesearch determines a step  $\alpha_k$  (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

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

where  $e = (1, 1, \dots, 1)^T$ . 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  $\pi$  for the nonlinear constraints become ‘large’) by solving a problem of the form

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

where

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

is called a *composite objective* and  $\gamma$  is a non-negative argument (the *elastic weight*). If  $\gamma$  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  $Sl_1$ QP algorithm of Fletcher (1984). See also Conn (1973).

## 12 Optional Arguments

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 arguments 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 Argument 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  $\epsilon$  is a generic notation for *machine precision* (see `nag_machine_precision` (X02AJC)).

<code>Nag_Start</code> start	<code>Nag_Cold</code>
Boolean list	<code>Nag_TRUE</code>
Boolean print_80ch	<code>Nag_TRUE</code>
<code>Nag_PrintType</code> print_level	<code>Nag_Soln_Iter</code>
<code>Nag_PrintType</code> minor_print_level	<code>Nag_NoPrint</code>
<code>Nag_DPrintType</code> print_deriv	<code>Nag_D.Print</code>
char outfile[80]	stdout
char **crnames	<b>NULL</b>
Boolean obj_deriv	<code>Nag_TRUE</code>
Boolean con_deriv	<code>Nag_TRUE</code>
<code>Nag_GradChk</code> verify_grad	<code>Nag_SimpleCheck</code>
Integer obj_check_start	1
Integer obj_check_stop	<b>nonln</b>
Integer con_check_start	1
Integer con_check_stop	<b>njnl</b>
double f_diff_int	$\sqrt{\text{options.f\_prec}}$
double c_diff_int	$\text{options.f\_prec}^{0.33}$
<code>Nag_CrashType</code> crash	<code>Nag_NoCrash</code> or <code>Nag_CrashThreeTimes</code>
Integer expand_freq	10000
Integer factor_freq	50 or 100
Integer fcheck	60
Integer hess_freq	9999999
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	$\max(\mathbf{options.inf\_bound}, 10^{20})$
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 Arguments

**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 arguments **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.

**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 <b>options.scale_opt</b> = 1 or 2; see below), basis factorization statistics and details of the initial basis resulting from the Crash procedure (if <b>options.start</b> = Nag_Cold and <b>options.crash</b> ≠ 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 ( $\leq 80$  characters);

if **options.print\_80ch** = Nag\_FALSE, one long line of output ( $\leq 120$  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 argument **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  $j$ th column (variable), for  $j = 1, 2, \dots, \mathbf{n}$ , and **options.crnames**[ $\mathbf{n} + i - 1$ ] contains the names of the  $i$ th row (constraint), for  $i = 1, 2, \dots, \mathbf{m}$ . If supplied, the names are used in the solution output (see Section 9.1 and Section 12.3).

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

**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 <b>objfun</b> and two calls to <b>confun</b> . 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 <b>options.print_deriv</b> = 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 of the constraint gradient (Jacobian) will be checked using a reliable (but more expensive) test. If <b>options.print_deriv</b> = 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 arguments **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 **njln**.

*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:*  $1 \leq \text{options.obj\_check\_start} \leq \text{options.obj\_check\_stop} \leq \text{nonln}$ .

**con\_check\_start** – Integer Default = 1  
**con\_check\_stop** – Integer Default = **njln**

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:*  $1 \leq \text{options.con\_check\_start} \leq \text{options.con\_check\_stop} \leq \text{njnl}$ .

**f\_diff\_int** – double Default =  $\sqrt{\text{options.f\_prec}}$

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 argument **options.verify\_grad**).
- (b) For estimating unspecified elements of the objective and/or the constraint Jacobian matrix.

Using the notation  $r = \text{options.f\_diff\_int}$ , a derivative with respect to  $x_j$  is estimated by perturbing that element of  $x$  to the value  $x_j + r(1 + |x_j|)$ , 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  $O(r)$ . 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:*  $\epsilon \leq \text{options.f\_diff\_int} < 1.0$ .

**c\_diff\_int** – double Default =  $\text{options.f\_prec}^{0.33}$

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 argument **options.f\_diff\_int**). Using the notation  $r = \text{options.c\_diff\_int}$ , the interval used for the  $j$ th variable is  $h_j = r(1 + |x_j|)$ . If the functions are well scaled, the resultant gradient estimates should be accurate to  $O(r^2)$ . 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:*  $\epsilon \leq \text{options.c\_diff\_int} < 1.0$ .

**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  $(A \ -I)$ . 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 = 1000

*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  $\delta$ . 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  $\delta$  (in steps of  $0.5\delta/\text{options.expand\_freq}$ ).

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**  $\geq 0$ .

**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 argument **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**  $\geq 0$ .

**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**  $\geq$  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**  $\geq$  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**  $\geq$  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**  $\geq$  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.

<b>options.part_price</b>	<b>Meaning</b>
1	All columns of the constraint matrix $(A \ -I)$ are searched.
$\geq 2$	Both $A$ and $I$ are partitioned to give <b>options.part_price</b> roughly equal segments $A_j, I_j$ , for $j = 1, 2, \dots, p$ (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  $\bar{a}_{ij} = a_{ij} \times (c_j/r_i)$  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.

<b>options.scale_opt</b>	<b>Meaning</b>
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 $(A \ -I)$ 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  $\bar{n} = \max(\mathbf{nonln}, \mathbf{njln})$ ), 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  $j$ th column, other nonzeros  $a_{ij}$  in the column are ignored if  $|a_{ij}| \leq a_{\max} \times \mathbf{options.crash\_tol}$ .



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:*  $0.0 \leq \text{options.crash\_tol} < 1.0$ .

**elastic\_wt** – double

Default = 1.0 or 100.0

*On entry:* this option defines the initial weight  $\gamma$  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**  $\times (1 + \|g(x_k)\|_2)$ , where  $g$  is the objective gradient. In either case, the QP subproblem is re-solved in elastic mode with  $\gamma = \text{options.elastic\_wt} \times (1 + \|g(x_k)\|_2)$ .

*Constraint:* **options.elastic\_wt**  $\geq 0.0$ .

**f\_prec** – double

Default =  $\epsilon^{0.8}$

*On entry:* this option defines the *relative function precision*  $\epsilon_R$ , 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  $\epsilon_R$  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,  $\epsilon_R$  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  $\epsilon_R$  would be  $10^{-10}$ .

The choice of  $\epsilon_R$  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:*  $\epsilon \leq \text{options.f\_prec} < 1.0$ .

**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  $-\text{options.inf\_bound}$  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:*  $0.0 \leq \text{options.linesearch\_tol} < 1.0$ .

**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**  $\geq 0.0$ .

**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  $|u_{jj}| \leq \text{options.lu\_sing\_tol}$  or  $|u_{jj}| < \text{options.lu\_sing\_tol} \times \max_i |u_{ij}|$ , the *j*th 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  $\mu$  satisfy  $|\mu| < \text{options.lu\_factor\_tol}$  during refactorization or  $|\mu| < \text{options.lu\_update\_tol}$  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:

$$\begin{aligned} \text{options.lu\_factor\_tol} &\geq 1.0; \\ \text{options.lu\_update\_tol} &\geq 1.0. \end{aligned}$$

**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

$$\text{rowerr} = \max_i \frac{\text{viol}_i}{\|(x, s)\|} \leq \text{options.major\_feas\_tol},$$

where  $\text{viol}_i$  is the violation of the  $i$ th 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  $(x, s, \pi)$  will have been computed such that

$$\text{maxgap} = \max_j \frac{\text{gap}_j}{\|\pi\|} \leq \text{options.major\_opt\_tol},$$

where  $\text{gap}_j$  is an estimate of the complementarity gap for the  $j$ th variable and  $\|\pi\|$  is a measure of the size of the QP dual variables (or Lagrange multipliers) given by

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

It is included to make the tests independent of a scale factor on the objective function. Specifically,  $\text{gap}_j$  is computed from the final QP solution using the reduced gradients  $d_j = g_j - \pi^T a_j$ , where  $g_j$  is the  $j$ th element of the objective gradient and  $a_j$  is the associated column of the constraint matrix  $(A \ -I)$ :

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

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  $\alpha$  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 argument **options.major\\_step\\_lim** is therefore used to define a step limit  $\bar{\beta}$  given by

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

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

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  $S_{\text{inf}}$  be the corresponding sum of infeasibilities. If  $S_{\text{inf}}$  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**  $\geq 1$ , 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  $d_j = g_j - \pi^T a_j$ , where  $g_j$  is the  $j$ th element of the QP gradient,  $a_j$  is the associated column of the QP constraint matrix and  $\pi$  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

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

respectively, and if  $\frac{|d_j|}{\|\pi\|} \leq \mathbf{options.minor\_opt\_tol}$  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 argument **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 approximately  $\mathbf{nnz} \times \mathbf{options.nz\_coef}$  reals and  $2 \times \mathbf{nnz} \times \mathbf{options.nz\_coef}$  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**  $\geq 1.0$ .

**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 argument **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 argument **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  $p$ th scaling pass through  $A$ . The scaling procedure is terminated if  $a_p \geq a_{p-1} \times \mathbf{options.scale\_tol}$  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:*  $0.0 < \mathbf{options.scale\_tol} < 1.0$ .

**unbounded\_obj** – double

Default =  $10^{15}$

**inf\_step** – double

Default =  $\max(\mathbf{options.inf\_bound}, 10^{20})$

*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  $\alpha$  varies. If  $|f|$  exceeds **options.unbounded\_obj** or  $\alpha$  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

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

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

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  $\alpha_k$ . 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  $\bar{n}$  ( $= \max(\mathbf{nonln}, \mathbf{njnln})$ ) < 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  $\pi_i$  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 argument **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  $(A \quad -I)$ . Possible values for **options.state**[ $j - 1$ ], for  $j = 1, 2, \dots, \mathbf{n}$ , 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  $j = 1, 2, \dots, \mathbf{n}$ . All variables will then be eligible for the initial basis. Less trivially, to say that the  $j$ th 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,  $0 \leq \mathbf{options.state}[j - 1] \leq 5$ , for  $j = 1, 2, \dots, \mathbf{n}$ ;
- if **options.start** = Nag\_Warm,  $0 \leq \mathbf{options.state}[j - 1] \leq 3$ , for  $j = 1, 2, \dots, \mathbf{n} + \mathbf{m}$ .

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

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

If the problem is feasible (i.e., **ninf** = 0), basic and superbasic variables may be outside their bounds by as much as the optional argument **options.minor\_feas\_tol**. Note that unless the optional argument **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 **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.

When a ‘warm start’ is chosen **options.lambda**[ $j - 1$ ] must contain a multiplier estimate for each nonlinear constraint for  $j = \mathbf{n} + 1, \mathbf{n} + 2, \dots, \mathbf{n} + \mathbf{ncnln}$ . 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  $j = \mathbf{n} + 1, \mathbf{n} + 2, \dots, \mathbf{n} + \mathbf{ncnln}$ .

*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 **m** – **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 argument **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:

<code>x[j-1]</code>	the element of $x$ .
<code>dx[j-1]</code>	the finite difference interval.
Jacobian value	the nonlinear Jacobian element.
<code>g[j-1]</code>	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 ( $\leq 120$  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 <b>objfun</b> 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 <b>confun</b> has been called to evaluate the nonlinear constraint functions (not printed if <b>ncnln</b> is zero).

Merit	<p>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 arguments (see Section 11.1). As the solution is approached, Merit will converge to the value of the objective function at the solution.</p> <p>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 argument <b>options.elastic_wt</b> (default value = 1.0 or 100.0).</p> <p>If there are no nonlinear constraints present, this entry contains Objective, the value of the objective function <math>f(x)</math>. In this case, <math>f(x)</math> will decrease monotonically to its optimal value.</p>
Feasibl	<p>is the value of <i>rowerr</i>, the largest element of the scaled nonlinear constraint residual vector defined in the description of the optional argument <b>options.major_feas_tol</b>. The solution is regarded as ‘feasible’ if Feasibl is less than (or equal to) <b>options.major_feas_tol</b> (default value = <math>\sqrt{\epsilon}</math>). Feasibl will be approximately zero in the neighbourhood of a solution.</p> <p>If there are no nonlinear constraints present, all iterates are feasible and this entry is not printed.</p>
Optimal	<p>is the value of <i>maxgap</i>, the largest element of the maximum complementarity gap vector defined in the description of the optional argument <b>options.major_opt_tol</b>. The Lagrange multipliers are regarded as ‘optimal’ if Optimal is less than (or equal to) <b>options.major_opt_tol</b> (default value = <math>\sqrt{\epsilon}</math>). Optimal will be approximately zero in the neighbourhood of a solution.</p>
nS	is the current number of superbasic variables.
Penalty	is the Euclidean norm of the vector of penalty arguments used in the augmented Lagrangian function (not printed if <b>ncnl</b> is zero).
LU	<p>is the number of nonzeros representing the basis factors <math>L</math> and <math>U</math> on completion of the QP subproblem.</p> <p>If there are nonlinear constraints present, the basis factorization <math>B = LU</math> is computed at the start of the first minor iteration. At this stage, <math>LU = \text{lenL} + \text{lenU}</math>, where <math>\text{lenL}</math> is the number of subdiagonal elements in the columns of a lower triangular matrix and <math>\text{lenU}</math> is the number of diagonal and superdiagonal elements in the rows of an upper triangular matrix. As columns of <math>B</math> 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 <math>LU</math> factors at the start of each QP subproblem.</p> <p>If there are no nonlinear constraints present, refactorization is subject only to the value of the optional argument <b>options.factor_freq</b> (default value = 50 or 100) and hence LU will tend to increase between factorizations.</p>
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 <b>ncnl</b> is zero). The swaps are determined by an $LU$ factorization of the rectangular matrix $B_S = (B \ S)^T$ , 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 <b>ncnl</b> and <b>nonln</b> 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 $R^T R$ 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 arguments <b>options.major_feas_tol</b> and <b>options.major_opt_tol</b> . 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 arguments **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 argument **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 argument **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 ( $\leq 80$  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 ( $\leq 120$  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 $\alpha$ 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 $r$ th element of a vector $y$ satisfying $By = a_q$ whenever $a_q$ (the $q$ th column of the constraint matrix $(A \ -I)$ ) replaces the $r$ th 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 argument <b>options.pivot_tol</b> (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 `ncnl` 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  $R^T R$  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 ( $\leq 120$  characters) are sent to `options.outfile` whenever the matrix  $B$  or  $B_S = (B \ S)^T$  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 argument `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 argument <code>options.factor_freq</code> (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 argument <code>options.fcheck</code> ).
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).
Elms	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, $\text{Density} = 100 \times \text{Elms} / (\text{Nonlinear} + \text{Linear} + \text{Slacks})^2$ .
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, $\text{Increase} = 100 \times (\text{lenL} + \text{lenU} - \text{Elms}) / \text{Elms}$ .
$m$	is the number of rows in the problem. Note that $m = U_t + L_t + \text{bp}$ .
$U_t$	is the number of triangular rows of $B$ at the top of $U$ .
$d_1$	is the number of columns remaining when the density of the basis matrix being factorized reached 0.3.
$L_{\max}$	is the maximum subdiagonal element in the columns of $L$ . This will not exceed the value of the optional argument <b>options.lu_factor_tol</b> (default value = 5.0 or 100.0).
$B_{\max}$	is the maximum nonzero element in $B$ (not printed if $B_S$ is factorized).
$BS_{\max}$	is the maximum nonzero element in $B_S$ (not printed if $B$ is factorized).
$U_{\max}$	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 $U_{\max}$ . If the basis is strictly triangular, <i>none</i> of the elements of $B$ will contribute, and $U_{\max}$ will be zero.)  Ideally, $U_{\max}$ should not be significantly larger than $B_{\max}$ . If it is several orders of magnitude larger, it may be advisable to reset the <b>options.lu_factor_tol</b> to some value nearer unity.  $U_{\max}$ is not printed if $B_S$ is factorized.
$U_{\min}$	is the magnitude of the smallest diagonal element of $PUQ$ .
Growth	is the value of the ratio $U_{\max}/B_{\max}$ , which should not be too large.  Providing $L_{\max}$ is not large (say $< 10.0$ ), the ratio $\max(B_{\max}, U_{\max})/U_{\min}$ 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 $U_{\min}$ extremely small, and the modified basis is refactored.)
$L_t$	is the number of triangular columns of $B$ at the left of $L$ .
$\text{bp}$	is the size of the ‘bump’ or block to be factorized nontrivially after the triangular rows and columns of $B$ have been removed.
$d_2$	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., <b>options.state</b> [ $j - 1$ ] = 3 for some $j \leq n$ ). It will be a subset of the columns for which <b>options.state</b> [ $j - 1$ ] = 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 ( $\leq 120$  characters) are sent to **options.outfile**.

Let  $x_j$  denote the  $j$ th ‘column variable’, for  $j = 1, 2, \dots, n$ . 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 $\alpha$ and $\beta$ . The various possible states are as follows:
LL	$x_j$ is nonbasic at its lower limit, $\alpha$ .
UL	$x_j$ is nonbasic at its upper limit, $\beta$ .
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 argument **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 argument **options.minor\_feas\_tol** (default value =  $\sqrt{\epsilon}$ ).

N	<i>Not precisely optimal.</i> $x_j$ is nonbasic. Its reduced gradient is larger than the value of the optional argument <b>options.major_feas_tol</b> (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 $\alpha$ , the lower bound specified for $x_j$ . None indicates that <b>bl</b> [ $j - 1$ ] $\leq$ <b>options.inf_bound</b> .
Upper Limit	is $\beta$ , the upper bound specified for $x_j$ . None indicates that <b>bu</b> [ $j - 1$ ] $\geq$ <b>options.inf_bound</b> .
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  $i$ th row of  $A$ , for  $i = 1, 2, \dots, n$ . The  $i$ th constraint is therefore of the form  $\alpha \leq a_i^T x \leq \beta$ , and the value of  $a_i^T x$  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  $i$ th '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  $\alpha \leq F_i(x) + a_i^T x \leq \beta$  are treated similarly, except that the row activity and degree of infeasibility are computed directly from  $F_i(x) + a_i^T x$  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 $i$ th row.
State	gives the state of the $i$ th row relative to the bounds $\alpha$ and $\beta$ . The various possible states are as follows:
LL	The row is at its lower limit, $\alpha$ .
UL	The row is at its upper limit, $\beta$ .
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 argument **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	<i>Alternative optimum possible.</i> $s_i$ 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 <i>might</i> change, giving a genuine alternative solution. The values of the dual variables (or Lagrange multipliers) <i>might</i> also change.
D	<i>Degenerate.</i> $s_i$ is basic, but it is equal to (or very close to) one of its bounds.
I	<i>Infeasible.</i> $s_i$ is basic and is currently violating one of its bounds by more than the value of the optional argument <b>options.minor_feas_tol</b> (default value = $\sqrt{\epsilon}$ ).
N	<i>Not precisely optimal.</i> $s_i$ is nonbasic. Its reduced gradient is larger than the value of the optional argument <b>options.major_feas_tol</b> (default value = $\sqrt{\epsilon}$ ).
Activity	is the value of $a_i^T x$ (or $F_i(x) + a_i^T x$ 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  $\alpha$ , the lower bound specified for the  $i$ th row. None indicates that  $\mathbf{bl}[n + i - 1] \leq -\mathbf{options.inf\_bound}$ .

Upper Limit is  $\beta$ , the upper bound specified for the  $i$ th row. None indicates that  $\mathbf{bu}[n + i - 1] \geq \mathbf{options.inf\_bound}$ .

Dual Activity is the value of the dual variable  $\pi_i$ .

$i$  gives the index  $i$  of the  $i$ th row.

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

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