

# NAG Library Function Document

## nag\_opt\_sparse\_convex\_qp (e04nkc)

### 1 Purpose

nag\_opt\_sparse\_convex\_qp (e04nkc) solves sparse linear programming or convex quadratic programming problems.

### 2 Specification

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

void nag_opt_sparse_convex_qp (Integer n, Integer m, Integer nnz,
    Integer iobj, Integer ncolh,
    void (*qphx)(Integer ncolh, const double x[], double hx[],
        Nag_Comm *comm),
    const double a[], const Integer ha[], const Integer ka[],
    const double bl[], const double bu[], double xs[], Integer *ninf,
    double *sinf, double *obj, Nag_E04_Opt *options, Nag_Comm *comm,
    NagError *fail)
```

### 3 Description

nag\_opt\_sparse\_convex\_qp (e04nkc) is designed to solve a class of quadratic programming problems that are assumed to be stated in the following general form:

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

where  $x$  is a set of variables,  $A$  is an  $m$  by  $n$  matrix and the objective function  $f(x)$  may be specified in a variety of ways depending upon the particular problem to be solved. The optional argument **options.minimize** (see Section 12.2) may be used to specify an alternative problem in which  $f(x)$  is maximized. The possible forms for  $f(x)$  are listed in Table 1 below, in which the prefixes FP, LP and QP stand for ‘feasible point’, ‘linear programming’ and ‘quadratic programming’ respectively,  $c$  is an  $n$  element vector and  $H$  is the  $n$  by  $n$  second-derivative matrix  $\nabla^2 f(x)$  (the *Hessian matrix*).

Problem Type	Objective Function $f(x)$	Hessian Matrix $H$
FP	Not applicable	Not applicable
LP	$c^T x$	Not applicable
QP	$c^T x + \frac{1}{2} x^T H x$	Symmetric positive semidefinite

Table 1

For LP and QP problems, the unique global minimum value of  $f(x)$  is found. For FP problems,  $f(x)$  is omitted and the function attempts to find a feasible point for the set of constraints. For QP problems, a function must also be provided to compute  $Hx$  for any given vector  $x$ . ( $H$  need not be stored explicitly.)

nag\_opt\_sparse\_convex\_qp (e04nkc) is intended to solve large-scale linear and quadratic programming problems in which the constraint matrix  $A$  is *sparse* (i.e., when the number of zero elements is sufficiently large that it is worthwhile using algorithms which avoid computations and storage involving zero elements). nag\_opt\_sparse\_convex\_qp (e04nkc) also takes advantage of sparsity in  $c$ . (Sparsity in  $H$  can be exploited in the function that computes  $Hx$ .) For problems in which  $A$  can be treated as a *dense* matrix, it is usually more efficient to use nag\_opt\_lp (e04mfc), nag\_opt\_lin\_lsq (e04ncc) or nag\_opt\_qp (e04nfc).

If  $H$  is positive definite, then the final  $x$  will be unique. If `nag_opt_sparse_convex_qp` (e04nkc) detects that  $H$  is indefinite, it terminates immediately with an error condition (see Section 6). In that case, it may be more appropriate to call `nag_opt_nlp_sparse` (e04ugc) instead. If  $H$  is the zero matrix, the function will still solve the resulting LP problem; however, this can be accomplished more efficiently by setting the argument `ncolh` = 0 (see Section 5).

The upper and lower bounds on the  $m$  elements of  $Ax$  are said to define the *general constraints* of the problem. Internally, `nag_opt_sparse_convex_qp` (e04nkc) converts the general constraints 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:

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

Since the slack variables  $s$  are subject to the same upper and lower bounds as the elements of  $Ax$ , the bounds on  $Ax$  and  $x$  can simply be thought of as bounds on the combined vector  $(x, s)$ . (In order to indicate their special role in QP problems, the original variables  $x$  are sometimes known as ‘column variables’, and the slack variables  $s$  are known as ‘row variables’.)

Each LP or QP problem is solved using an *active-set* method. This is an iterative procedure with two phases: a *feasibility phase*, in which the sum of infeasibilities is minimized to find a feasible point; and an *optimality phase*, in which  $f(x)$  is minimized by constructing a sequence of iterations that lies within the feasible region.

A constraint is said to be *active* or *binding* at  $x$  if the associated element of either  $x$  or  $Ax$  is equal to one of its upper or lower bounds. Since an active constraint in  $Ax$  has its associated slack variable at a bound, the status of both simple and general upper and lower bounds can be conveniently described in terms of the status of the variables  $(x, s)$ . A variable is said to be *nonbasic* if it is temporarily fixed at its upper or lower bound. It follows that regarding a general constraint as being *active* is equivalent to thinking of its associated slack as being *nonbasic*.

At each iteration of an active-set method, the constraints  $Ax - s = 0$  are (conceptually) partitioned into the form

$$Bx_B + Sx_S + Nx_N = 0,$$

where  $x_N$  consists of the nonbasic elements of  $(x, s)$  and the *basis matrix*  $B$  is square and nonsingular. The elements of  $x_B$  and  $x_S$  are called the *basic* and *superbasic* variables respectively; with  $x_N$  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 upper or lower bounds, while the nonbasic variables will be equal to one of their bounds. At each iteration,  $x_S$  is regarded as a set of independent variables that are free to move in any desired direction, namely one that will improve the value of the objective function (or sum of infeasibilities). The basic variables are then adjusted in order to ensure that  $(x, s)$  continues to satisfy  $Ax - s = 0$ . The number of superbasic variables ( $n_S$  say) therefore indicates the number of degrees of freedom remaining after the constraints have been satisfied. In broad terms,  $n_S$  is a measure of *how nonlinear* the problem is. In particular,  $n_S$  will always be zero for FP and LP problems.

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

Associated with each of the  $m$  equality constraints  $Ax - s = 0$  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; and the reduced gradients for the slack variables  $s$  are the dual variables  $\pi$ . The QP subproblem is optimal if  $d_j \geq 0$  for all nonbasic variables at their lower bounds,  $d_j \leq 0$  for all nonbasic variables at their upper bounds and  $d_j = 0$  for all superbasic variables. In practice, an *approximate* QP solution is found by slightly relaxing these conditions on  $d_j$  (see the description of the optional argument `options.optim_tol` in Section 12.2).

The process of computing and comparing reduced gradients is known as *pricing* (a term first introduced in the context of the simplex method for linear programming). To ‘price’ a nonbasic variable  $x_j$  means that the reduced gradient  $d_j$  associated with the relevant active upper or lower bound on  $x_j$  is computed via the formula  $d_j = g_j - a_j^T \pi$ , where  $a_j$  is the  $j$ th column of  $(A \ -I)$ . (The variable selected by such a process and the corresponding value of  $d_j$  (i.e., its reduced gradient) are the quantities +S and dj in the detailed printed output from `nag_opt_sparse_convex_qp` (e04nkc); see Section 12.3.) If  $A$  has significantly more columns than rows (i.e.,  $n \gg m$ ), pricing can be computationally expensive. In this case, a strategy known as *partial pricing* can be used to compute and compare only a subset of the  $d_j$ 's.

`nag_opt_sparse_convex_qp` (e04nkc) is based on SQOPT, which is part of the SNOPT package described in Gill *et al.* (2002), which in turn utilizes routines from the MINOS package (see Murtagh and Saunders (1995)). It uses stable numerical methods throughout and includes a reliable basis package (for maintaining sparse  $LU$  factors of the basis matrix  $B$ ), a practical anti-degeneracy procedure, efficient handling of linear constraints and bounds on the variables (by an active-set strategy), as well as automatic scaling of the constraints. Further details can be found in Section 9.

## 4 References

- Fourer R (1982) Solving staircase linear programs by the simplex method *Math. Programming* **23** 274–313
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- Gill P E, Murray W and Saunders M A (2002) *SNOPT: An SQP Algorithm for Large-scale Constrained Optimization* **12** 979–1006 SIAM J. Optim.
- Gill P E, Murray W, Saunders M A and Wright M H (1987) Maintaining  $LU$  factors of a general sparse matrix *Linear Algebra and its Applics.* **88/89** 239–270
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- Hall J A J and McKinnon K I M (1996) The simplest examples where the simplex method cycles and conditions where EXPAND fails to prevent cycling *Report MS 96–100* Department of Mathematics and Statistics, University of Edinburgh
- Murtagh B A and Saunders M A (1995) MINOS 5.4 users' guide *Report SOL 83-20R* Department of Operations Research, Stanford University

## 5 Arguments

- 1: **n** – Integer *Input*  
*On entry:*  $n$ , the number of variables (excluding slacks). This is the number of columns in the linear constraint matrix  $A$ .  
*Constraint:*  $n \geq 1$ .
- 2: **m** – Integer *Input*  
*On entry:*  $m$ , the number of general linear constraints (or slacks). This is the number of rows in  $A$ , including the free row (if any; see argument **iobj**).  
*Constraint:*  $m \geq 1$ .
- 3: **nnz** – Integer *Input*  
*On entry:* the number of nonzero elements in  $A$ .  
*Constraint:*  $1 \leq \mathbf{nnz} \leq \mathbf{n} \times \mathbf{m}$ .

4: **iobj** – Integer *Input*

*On entry:* if **iobj** > 0, row **iobj** of  $A$  is a free row containing the nonzero elements of the vector  $c$  appearing in the linear objective term  $c^T x$ .

If **iobj** = 0, there is no free row – i.e., the problem is either an FP problem (in which case **iobj** must be set to zero), or a QP problem with  $c = 0$ .

*Constraint:*  $0 \leq \mathbf{iobj} \leq \mathbf{m}$ .

5: **ncolh** – Integer *Input*

*On entry:*  $n_H$ , the number of leading nonzero columns of the Hessian matrix  $H$ . For FP and LP problems, **ncolh** must be set to zero.

*Constraint:*  $0 \leq \mathbf{ncolh} \leq \mathbf{n}$ .

6: **qphx** – function, supplied by the user *External Function*

**qphx** must be supplied for QP problems to compute the matrix product  $Hx$ . If  $H$  has zero rows and columns, it is most efficient to order the variables  $x = (y \ z)^T$  so that

$$Hx = \begin{pmatrix} H_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix} = \begin{pmatrix} H_1 y \\ 0 \end{pmatrix},$$

where the nonlinear variables  $y$  appear first as shown. For FP and LP problems, **qphx** will never be called and the NAG defined null function pointer, NULLFN, can be supplied in the call to `nag_opt_sparse_convex_qp` (e04nkc).

The specification of **qphx** is:

```
void qphx (Integer ncolh, const double x[], double hx[],
          Nag_Comm *comm)
```

1: **ncolh** – Integer *Input*

*On entry:* the number of leading nonzero columns of the Hessian matrix  $H$ , as supplied to `nag_opt_sparse_convex_qp` (e04nkc).

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

*On entry:* the first **ncolh** elements of **x**.

3: **hx[ncolh]** – double *Output*

*On exit:* the product  $Hx$ .

4: **comm** – Nag\_Comm \*  
 Pointer to structure of type Nag\_Comm; the following members are relevant to **qphx**.

**first** – Nag\_Boolean *Input*

*On entry:* will be set to Nag\_TRUE on the first call to **qphx** and Nag\_FALSE for all subsequent calls.

**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 **qphx** including the current one.

**user** – double \*

**iuser** – Integer \*

**p** – Pointer

The type Pointer will be `void *` with a C compiler that defines `void *` or `char *`.

Before calling `nag_opt_sparse_convex_qp` (e04nkc) these pointers may be allocated memory and initialized with various quantities for use by `qphx` when called from `nag_opt_sparse_convex_qp` (e04nkc).

**Note:** `qphx` should be tested separately before being used in conjunction with `nag_opt_sparse_convex_qp` (e04nkc). The array `x` must **not** be changed by `qphx`.

7: `a[nnz]` – const double *Input*

*On entry:* the nonzero elements of  $A$ , ordered by increasing column index. Note that elements with the same row and column indices are not allowed. The row and column indices are specified by arguments `ha` and `ka` (see below).

8: `ha[nnz]` – const Integer *Input*

*On entry:* `ha[i]` must contain the row index of the nonzero element stored in `a[i]`, for  $i = 0, 1, \dots, \text{nnz} - 1$ . Note that the row indices for a column may be supplied in any order.

*Constraint:*  $1 \leq \text{ha}[i] \leq m$ , for  $i = 0, 1, \dots, \text{nnz} - 1$ .

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

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

*Constraints:*

`ka[0] = 0;`  
`ka[j - 1] ≥ 0`, for  $j = 2, 3, \dots, n$ ;  
`ka[n] = nnz;`  
 $0 \leq \text{ka}[j] - \text{ka}[j - 1] \leq m$ , for  $j = 1, 2, \dots, n$ .

10: `bl[n + m]` – const double *Input*

11: `bu[n + m]` – const double *Input*

*On entry:* `bl` must contain the lower bounds and `bu` the upper bounds, for all the constraints in the following order. The first  $n$  elements of each array must contain the bounds on the variables, and the next  $m$  elements the bounds for the general linear constraints  $Ax$  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] = β`, say, where  $|\beta| < \text{options.inf\_bound}$ . Note that, for LP and QP problems, the lower bound corresponding to the free row 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]`.

*Constraints:*

`bl[j] ≤ bu[j]`, for  $j = 0, 1, \dots, n + m - 1$ ;  
if `bl[j] = bu[j] = β`,  $|\beta| < \text{options.inf\_bound}$ ;  
if `iobj > 0`, `bl[n + iobj - 1] ≤ -options.inf_bound` and  
`bu[n + iobj - 1] ≥ options.inf_bound`.

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

*On entry:* `xs[j - 1]`, for  $j = 1, 2, \dots, n$ , 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[n + i - 1]`, for  $i = 1, 2, \dots, m$ , must contain the initial values of the slack variables,  $s$ .

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

- 13: **ninf** – Integer \* *Output*  
*On exit:* the number of infeasibilities. This will be zero if an optimal solution is found, i.e., if `nag_opt_sparse_convex_qp` (e04nkc) exits with **fail.code** = NE\_NOERROR or NW\_SOLN\_NOT\_UNIQUE.
- 14: **sinf** – double \* *Output*  
*On exit:* the sum of infeasibilities. This will be zero if **ninf** = 0. (Note that `nag_opt_sparse_convex_qp` (e04nkc) does attempt to compute the minimum value of **sinf** in the event that the problem is determined to be infeasible, i.e., when `nag_opt_sparse_convex_qp` (e04nkc) exits with **fail.code** = NW\_NOT\_FEASIBLE.)
- 15: **obj** – double \* *Output*  
*On exit:* the value of the objective function.  
 If **ninf** = 0, **obj** includes the quadratic objective term  $\frac{1}{2}x^T Hx$  (if any).  
 If **ninf** > 0, **obj** is just the linear objective term  $c^T x$  (if any).  
 For FP problems, **obj** is set to zero.
- 16: **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_sparse_convex_qp` (e04nkc). 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_sparse_convex_qp` (e04nkc) to perform a ‘warm start’ (see the member **options.start** in Section 12.2).  
 The **options** structure also allows names to be assigned to the columns and rows (i.e., the variables and constraints) of the problem, which are then used in solution output.  
 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_sparse_convex_qp` (e04nkc). However, if the optional arguments are not required the NAG defined null pointer, E04\_DEFAULT, can be used in the function call.
- 17: **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 function, **qphx**, and the optional user-defined printing function; see the description of **qphx** and Section 12.3.1 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_sparse_convex_qp` (e04nkc); **comm** will then be declared internally for use in calls to user-supplied functions.
- 18: **fail** – NagError \* *Input/Output*  
 The NAG error argument (see Section 3.6 in the Essential Introduction).

## 5.1 Description of Printed Output

Intermediate and final results are printed out by default. The level of printed output can be controlled with the structure member **options.print.level** (see Section 12.2). The default, **options.print.level** = Nag\_Soln\_Iter, provides a single line of output at each iteration and the final result. This section describes the default printout produced by `nag_opt_sparse_convex_qp` (e04nkc).

The following line of summary output (< 80 characters) is produced at every iteration. In all cases, 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 violated constraints (infeasibilities). This will be zero during the optimality phase.
Sinf/Objective	is the current value of the objective function. If $x$ is not feasible, Sinf gives the sum of magnitudes of constraint violations. If $x$ is feasible, Objective is the value of the objective function. The output line for the final iteration of the feasibility phase (i.e., the first iteration for which Ninf is zero) will give the value of the true objective at the first feasible point.

During the optimality phase, the value of the objective function will be non-increasing. During the feasibility phase, the number of constraint infeasibilities will not increase until either a feasible point is found, or the optimality of the multipliers implies that no feasible point exists.

Norm rg	is $\ d_S\ $ , the Euclidean norm of the reduced gradient (see Section 11.3). During the optimality phase, this norm will be approximately zero after a unit step. For FP and LP problems, Norm rg is not printed.
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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 variable $j$ , for $j = 1, 2, \dots, n$ . If an <b>options</b> structure is supplied to nag_opt_sparse_convex_qp (e04nkc), and the <b>options.crnames</b> member is assigned to an array of column and row names (see Section 12.2 for details), the name supplied in <b>options.crnames</b> [ $j - 1$ ] is assigned to the $j$ th variable. Otherwise, a default name is assigned to the variable.
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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).
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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** = Nag\_NoScale (default value is **options.scale** = Nag\_ExtraScale; see Section 12.2) 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 bound, there would be no change in the value of the objective function. The values of the other free variables *might* change, giving a genuine alternative solution. However, if there are any degenerate variables (labelled D), the actual change might prove to be zero, since one of them could encounter a bound immediately. In either case, the values of the Lagrange multipliers *might* also change.

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

I *Infeasible*. The variable is basic or superbasic and is currently violating one of its bounds by more than the value of the optional argument **options.ftol** (default value =  $\max(10^{-6}, \sqrt{\epsilon})$ , where  $\epsilon$  is the *machine precision*; see Section 12.2).

N *Not precisely optimal*. The variable is nonbasic or superbasic. If the value of the reduced gradient for the variable exceeds the value of the optional argument **options.optim\_tol** (default value =  $\max(10^{-6}, \sqrt{\epsilon})$ ; see Section 12.2), the solution would not be declared optimal because the reduced gradient for the variable would not be considered negligible.

Value	is the value of the variable at the final iteration.
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Lower Bound	is the lower bound specified for variable $j$ . (None indicates that $\mathbf{bl}[j-1] \leq -\mathbf{options.inf\_bound}$ , where $\mathbf{options.inf\_bound}$ is the optional argument.)
Upper Bound	is the upper bound specified for variable $j$ . (None indicates that $\mathbf{bu}[j-1] \geq \mathbf{options.inf\_bound}$ .)
Lagr Mult	is the value of the Lagrange multiplier for the associated bound. This will be zero if State is FR. If $x$ is optimal, the multiplier should be non-negative if State is LL, non-positive if State is UL, and zero if State is BS or SBS.
Residual	is the difference between the variable Value and the nearer of its (finite) bounds $\mathbf{bl}[j-1]$ 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  $m$ ,  $\mathbf{options.cnames}[j-1]$  replaced by  $\mathbf{options.cnames}[n+j-1]$ ,  $\mathbf{bl}[j-1]$  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 linear constraint.

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

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\_ALLOC\_FAIL

Dynamic memory allocation failed.

### NE\_ARRAY\_CONS

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

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

### NE\_BAD\_PARAM

On entry, argument  $\mathbf{options.crash}$  had an illegal value.

On entry, argument  $\mathbf{options.print\_level}$  had an illegal value.

On entry, argument  $\mathbf{options.scale}$  had an illegal value.

On entry, argument  $\mathbf{options.start}$  had an illegal value.

### NE\_BASIS\_ILL\_COND

Numerical error in trying to satisfy the general constraints. The basis is very ill conditioned.

### NE\_BASIS\_SINGULAR

The basis is singular after 15 attempts to factorize it.

The basis is singular after 15 attempts to factorize it (adding slacks where necessary). Either the problem is badly scaled or the value of the optional argument  $\mathbf{options.lu\_factor\_tol}$  is too large; see Section 12.2.



**NE\_BOUND**

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

**NE\_BOUND\_EQ**

The lower bound and upper bound for variable  $\langle value \rangle$  (array elements  $\mathbf{bl}[\langle value \rangle]$  and  $\mathbf{bu}[\langle value \rangle]$ ) 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 elements  $\mathbf{bl}[\langle value \rangle]$  and  $\mathbf{bu}[\langle value \rangle]$ ) 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  $\mathbf{bl}[\langle value \rangle]$ ) is greater than the upper bound.

**NE\_DUPLICATE\_ELEMENT**

Duplicate sparse matrix element found in row  $\langle value \rangle$ , column  $\langle value \rangle$ .

**NE\_HESS\_INDEF**

The Hessian matrix  $H$  appears to be indefinite.

The Hessian matrix  $Z^T H Z$  (see Section 11.2) appears to be indefinite – normally because  $H$  is indefinite. Check that function **qphx** has been coded correctly. If **qphx** is coded correctly with  $H$  symmetric positive (semi-)definite, then the problem may be due to a loss of accuracy in the internal computation of the reduced Hessian. Try to reduce the values of the optional arguments **options.lu\_factor\_tol** and **options.lu\_update\_tol** (see Section 12.2).

**NE\_HESS\_TOO\_BIG**

Reduced Hessian exceeds assigned dimension. **options.max\_sb** =  $\langle value \rangle$ .

The reduced Hessian matrix  $Z^T H Z$  (see Section 11.2) exceeds its assigned dimension. The value of the optional argument **options.max\_sb** is too small; see Section 12.2.

**NE\_INT\_ARG\_LT**

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  $\mathbf{ka}[\langle value \rangle]$  not valid. Correct range for elements of **ka** is  $\geq 0$ .

**NE\_INT\_ARRAY\_2**

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

**NE\_INT\_OPT\_ARG\_LT**

On entry, **options.factor\_freq** =  $\langle value \rangle$ .  
Constraint: **options.factor\_freq**  $\geq$  1.

On entry, **options.fcheck** =  $\langle value \rangle$ .  
Constraint: **options.fcheck**  $\geq$  1.

On entry, **options.max\_iter** =  $\langle value \rangle$ .  
Constraint: **options.max\_iter**  $\geq$  0.

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

Constraint: **options.max\_sb**  $\geq 1$ .

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

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

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

Constraint: **options.partial\_price**  $\geq 1$ .

### NE\_INTERNAL\_ERROR

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please contact NAG for assistance.

### NE\_INVALID\_INT\_RANGE\_1

Value  $\langle value \rangle$  given to **iobj** is not valid. Correct range is  $0 \leq \mathbf{iobj} \leq \mathbf{m}$ .

Value  $\langle value \rangle$  given to **ncolh** is not valid. Correct range is  $0 \leq \mathbf{ncolh} \leq \mathbf{n}$ .

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

### NE\_INVALID\_INT\_RANGE\_2

Value  $\langle value \rangle$  given to **options.reset\_ftol** is not valid. Correct range is

$0 < \mathbf{options.reset\_ftol} < 10000000$ .

### NE\_INVALID\_REAL\_RANGE\_F

Value  $\langle value \rangle$  given to **options.ftol** is not valid. Correct range is **options.ftol**  $\geq \epsilon$ .

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\_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.optim\_tol** is not valid. Correct range is **options.optim\_tol**  $\geq \epsilon$ .

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

### NE\_INVALID\_REAL\_RANGE\_FF

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

Value  $\langle value \rangle$  given to **options.scale\_tol** is not valid. Correct range is  $0.0 < \mathbf{options.scale\_tol} < 1.0$ .

### NE\_NAME\_TOO\_LONG

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

### NE\_NOT\_APPEND\_FILE

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

### NE\_NOT\_CLOSE\_FILE

Cannot close file  $\langle string \rangle$ .

**NE\_NULL\_QPHX**

Since argument **ncolh** is nonzero, the problem is assumed to be of type QP. However, the argument **qphx** is a null function. **qphx** must be non-null for QP problems.

**NE\_OBJ\_BOUND**

Invalid lower bound for objective row. Bound should be  $\leq \langle value \rangle$ .

Invalid upper bound for objective row. Bound should be  $\geq \langle value \rangle$ .

**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 `options.max_restart`, has been reached.

**NE\_STATE\_VAL**

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

**NE\_UNBOUNDED**

Solution appears to be unbounded.

The problem is unbounded (or badly scaled). The objective function is not bounded below in the feasible region.

**NE\_WRITE\_ERROR**

Error occurred when writing to file `⟨string⟩`.

**NW\_NOT\_FEASIBLE**

No feasible point was found for the linear constraints.

The problem is infeasible. The general constraints cannot all be satisfied simultaneously to within the value of the optional argument `options.ftol`; see Section 12.2.

**NW\_SOLN\_NOT\_UNIQUE**

Optimal solution is not unique.

Weak solution found. The final  $x$  is not unique, although  $x$  gives the global minimum value of the objective function.

**NW\_TOO\_MANY\_ITER**

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

Too many iterations. The value of the optional argument `options.max_iter` is too small; see Section 12.2.

**7 Accuracy**

`nag_opt_sparse_convex_qp` (e04nkc) implements a numerically stable active set strategy and returns solutions that are as accurate as the condition of the problem warrants on the machine.

**8 Parallelism and Performance**

Not applicable.

## 9 Further Comments

None.

## 10 Example

To minimize the quadratic function  $f(x) = c^T x + \frac{1}{2} x^T H x$ , where

$$c = (-200, -2000, -2000, -2000, -2000, 400, 400)^T$$

$$H = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 0 & 0 & 2 & 2 \end{pmatrix}$$

subject to the bounds

$$\begin{aligned} 0 &\leq x_1 \leq 200 \\ 0 &\leq x_2 \leq 2500 \\ 400 &\leq x_3 \leq 800 \\ 100 &\leq x_4 \leq 700 \\ 0 &\leq x_5 \leq 1500 \\ 0 &\leq x_6 \\ 0 &\leq x_7 \end{aligned}$$

and the general constraints

$$\begin{array}{rcccccccc} & x_1 + & x_2 + & x_3 + & x_4 + & x_5 + & x_6 + & x_7 = & 2000 \\ 0.15x_1 + & 0.04x_2 + & 0.02x_3 + & 0.04x_4 + & 0.02x_5 + & 0.01x_6 + & 0.03x_7 & \leq & 60 \\ 0.03x_1 + & 0.05x_2 + & 0.08x_3 + & 0.02x_4 + & 0.06x_5 + & 0.01x_6 & & \leq & 100 \\ 0.02x_1 + & 0.04x_2 + & 0.01x_3 + & 0.02x_4 + & 0.02x_5 & & & \leq & 40 \\ 0.02x_1 + & 0.03x_2 & & & + & 0.01x_5 & & \leq & 30 \\ 1500 \leq & 0.70x_1 + & 0.75x_2 + & 0.80x_3 + & 0.75x_4 + & 0.80x_5 + & 0.97x_6 & & \\ 250 \leq & 0.02x_1 + & 0.06x_2 + & 0.08x_3 + & 0.12x_4 + & 0.02x_5 + & 0.01x_6 + & 0.97x_7 & \leq & 300 \end{array}$$

The initial point, which is infeasible, is

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

The optimal solution (to five figures) is

$$x^* = (0.0, 349.40, 648.85, 172.85, 407.52, 271.36, 150.02)^T.$$

One bound constraint and four linear constraints are active at the solution. Note that the Hessian matrix  $H$  is positive semidefinite.

The function to calculate  $Hx$  (**qphx** in the argument list; see Section 5) is **qphess**.

The example program shows the use of the **options** and **comm** structures. The data for the example include a set of user-defined column and row names, and data for the Hessian in a sparse storage format (see Section 10.2 for further details).

The **options** structure is initialized by **nag\_opt\_init** (e04xxc) and the **options.cnames** member is assigned to the array of character strings into which the column and row names were read. The **comm**→**p** member of **comm** is used to pass the Hessian into **nag\_opt\_sparse\_convex\_qp** (e04nkc) for use by the function **qphess**.

On return from **nag\_opt\_sparse\_convex\_qp** (e04nkc), the Hessian data is perturbed slightly and two further options set, selecting a warm start and a reduced level of printout. **nag\_opt\_sparse\_convex\_qp** (e04nkc) 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_sparse_convex_qp` (e04nkc) to the pointers in the options structure. You must **not** use the standard C function `free()` for this purpose.

The sparse storage scheme used for the Hessian in this example is similar to that which `nag_opt_sparse_convex_qp` (e04nkc) uses for the constraint matrix **a**, but since the Hessian is symmetric we need only store the lower triangle (including the diagonal) of the matrix. Thus, an array `hess` contains the nonzero elements of the lower triangle arranged in order of increasing column index. The array `khess` contains the indices in `hess` of the first element in each column, and the array `hhess` contains the row index associated with each element in `hess`. To allow the data to be passed via the **comm**→**p** member of **comm**, a struct `HessianData` is declared, containing pointer members which are assigned to the three arrays defining the Hessian. Alternative approaches would have been to use the **comm**→**user** and **comm**→**iuser** members of **comm** to pass suitably partitioned arrays to `qphess`, or to avoid the use of **comm** altogether and declare the Hessian data as global. The storage scheme suggested here is for illustrative purposes only.

## 10.1 Program Text

```

/* nag_opt_sparse_convex_qp (e04nkc) Example Program.
 *
 * Copyright 2014 Numerical Algorithms Group.
 *
 * Mark 5, 1998.
 * Mark 6 revised, 2000.
 * Mark 7 revised, 2001.
 * Mark 8 revised, 2004.
 *
 */

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

#ifdef __cplusplus
extern "C" {
#endif
static void NAG_CALL qphess(Integer ncolh, const double x[], double hx[],
                             Nag_Comm *comm);
#ifdef __cplusplus
}
#endif

/* Declare a data structure for passing sparse Hessian data to qphess */
typedef struct
{
    double *hess;
    Integer *khess;
    Integer *hhess;
} HessianData;

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

int main(void)
{
    HessianData hess_data;
    Integer exit_status = 0, *ha = 0, *hhess = 0, i, icol, iobj, j, jcol;
    Integer *ka = 0, *khess = 0, m, n, nbnd, ncolh, ninf, nnz, nnz_hess;
    Nag_Comm comm;
    Nag_E04_Opt options;
    char **crnames = 0, *names = 0;
    double *a = 0, *bl = 0, *bu = 0, *hess = 0, obj, sinf, *x = 0;
    NagError fail;

    INIT_FAIL(fail);

    printf("nag_opt_sparse_convex_qp (e04nkc) Example Program Results\n");

```

```

    fflush(stdout);

    /* Skip heading in data file */
#ifdef _WIN32
    scanf_s(" %*[\n]");
#else
    scanf(" %*[\n]");
#endif
    /* Read the problem dimensions */
#ifdef _WIN32
    scanf_s(" %*[\n]");
#else
    scanf(" %*[\n]");
#endif
#ifdef _WIN32
    scanf_s("%"NAG_IFMT%"NAG_IFMT"", &n, &m);
#else
    scanf("%"NAG_IFMT%"NAG_IFMT"", &n, &m);
#endif

    /* Read nnz, iobj, ncolh */
#ifdef _WIN32
    scanf_s(" %*[\n]");
#else
    scanf(" %*[\n]");
#endif
#ifdef _WIN32
    scanf_s("%"NAG_IFMT%"NAG_IFMT%"NAG_IFMT"", &nnz, &iobj, &ncolh);
#else
    scanf("%"NAG_IFMT%"NAG_IFMT%"NAG_IFMT"", &nnz, &iobj, &ncolh);
#endif

    if (n >= 1 && m >= 1 && nnz >= 1 && nnz <= n*m)
    {
        nbnd = n + m;
        if (!(a = NAG_ALLOC(nnz, double)) ||
            !(b1 = NAG_ALLOC(nbnd, double)) ||
            !(bu = NAG_ALLOC(nbnd, double)) ||
            !(x = NAG_ALLOC(nbnd, double)) ||
            !(ha = NAG_ALLOC(nnz, Integer)) ||
            !(ka = NAG_ALLOC(n+1, Integer)) ||
            !(kness = NAG_ALLOC(n+1, Integer)) ||
            !(crnames = NAG_ALLOC(nbnd, char *)) ||
            !(names = NAG_ALLOC(nbnd*9, char))
        )
        {
            printf("Allocation failure\n");
            exit_status = -1;
            goto END;
        }
    }
    else
    {
        printf("Invalid n or m or nnz.\n");
        exit_status = 1;
        return exit_status;
    }

    /* Read the matrix and set up ka */
    jcol = 1;
    ka[jcol-1] = 0;
#ifdef _WIN32
    scanf_s(" %*[\n]");
#else
    scanf(" %*[\n]");
#endif
    for (i = 0; i < nnz; ++i)
    {
        /* a[i] stores the (ha[i], icol) element of matrix */
#ifdef _WIN32
        scanf_s("%lf%"NAG_IFMT%"NAG_IFMT"", &a[i], &ha[i], &icol);

```

```

#else
    scanf("%lf%"NAG_IFMT%"NAG_IFMT"", &a[i], &ha[i], &icol);
#endif

    /* Check whether we have started a new column */
    if (icol == jcol+1)
    {
        ka[icol-1] = i; /* Start of icol-th column in a */
        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; ++j)
            ka[j-1] = i;

        ka[icol-1] = i;
        jcol = icol;
    }
}
ka[n] = nnz;

/* If the last columns are empty, set ka accordingly */
if (n > icol)
{
    for (j = icol; j <= n - 1; ++j)
        ka[j] = nnz;
}

/* Read the bounds */
nbnd = n+m;
#ifdef _WIN32
    scanf_s("%*[\n]"); /* Skip heading in data file */
#else
    scanf("%*[\n]"); /* Skip heading in data file */
#endif
for (i = 0; i < nbnd; ++i)
#ifdef _WIN32
    scanf_s("%lf", &bl[i]);
#else
    scanf("%lf", &bl[i]);
#endif
#ifdef _WIN32
    scanf_s("%*[\n]");
#else
    scanf("%*[\n]");
#endif
for (i = 0; i < nbnd; ++i)
#ifdef _WIN32
    scanf_s("%lf", &bu[i]);
#else
    scanf("%lf", &bu[i]);
#endif

/* Read the column and row names */
#ifdef _WIN32
    scanf_s("%*[\n]"); /* Skip heading in data file */
#else
    scanf("%*[\n]"); /* Skip heading in data file */
#endif
#ifdef _WIN32
    scanf_s("%*[']");
#else
    scanf("%*[']");
#endif
for (i = 0; i < nbnd; ++i)
{

```

```

#ifdef _WIN32
    scanf_s(" '%8c'", &NAMES(i, 0), 9);
#else
    scanf(" '%8c'", &NAMES(i, 0));
#endif
    NAMES(i, 8) = '\setminus 0';
    crnames[i] = &NAMES(i, 0);
}

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

    /* Read nnz_hess */
#ifdef _WIN32
    scanf_s(" %*[\n]");
#else
    scanf(" %*[\n]");
#endif
#ifdef _WIN32
    scanf_s("%"NAG_IFMT"", &nnz_hess);
#else
    scanf("%"NAG_IFMT"", &nnz_hess);
#endif

    if (!(hess = NAG_ALLOC(nnz_hess, double)) ||
        !(hhess = NAG_ALLOC(nnz_hess, Integer)))
    {
        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }

    /* Read the hessian matrix and set up khess */
    jcol = 1;
    khess[jcol-1] = 0;
#ifdef _WIN32
    scanf_s(" %*[\n]");
#else
    scanf(" %*[\n]");
#endif
    for (i = 0; i < nnz_hess; ++i)
    {
        /* hess[i] stores the (hhess[i], icol) element of matrix */
#ifdef _WIN32
        scanf_s("%lf%"NAG_IFMT%"%"NAG_IFMT"", &hess[i], &hhess[i], &icol);
#else
        scanf("%lf%"NAG_IFMT%"%"NAG_IFMT"", &hess[i], &hhess[i], &icol);
#endif

        /* Check whether we have started a new column */
        if (icol == jcol+1)
        {
            khess[icol-1] = i; /* Start of icol-th column in hess */
            jcol = icol;
        }
        else if (icol > jcol+1)
        {
            /* Index in hess 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 khess to i.
            */

```



```

        */
        for (j = jcol+1; j < icol; ++j)
            khess[j-1] = i;

        khess[icol-1] = i;
    }
}
khess[ncolh] = nnz_hess;

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

/* Package up Hessian data for communication via comm */
hess_data.hess = hess;
hess_data.khess = khess;
hess_data.hhess = hhess;

comm.p = (Pointer)&hess_data;

/* Solve the problem */
/* nag_opt_sparse_convex_qp (e04nkc), see above. */
nag_opt_sparse_convex_qp(n, m, nnz, iobj, ncolh, qphess, a, ha, ka, bl, bu,
                        x, &ninf, &sinf, &obj, &options, &comm, &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_opt_sparse_convex_qp (e04nkc).\n%s\n",
           fail.message);
    exit_status = 1;
    goto END;
}

printf("\nPerturb the problem and re-solve with warm start.\n");
fflush(stdout);
for (i = 0; i < nnz_hess; ++i)
    hess[i] *= 1.001;

options.start = Nag_Warm;
options.print_level = Nag_Soln;
/* nag_opt_sparse_convex_qp (e04nkc), see above. */
nag_opt_sparse_convex_qp(n, m, nnz, iobj, ncolh, qphess, a, ha, ka, bl, bu,
                        x, &ninf, &sinf, &obj, &options, &comm, &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_opt_sparse_convex_qp (e04nkc).\n%s\n",
           fail.message);
    exit_status = 1;
    goto END;
}

/* Free memory NAG-allocated to members of options */
/* nag_opt_free (e04xzc).
 * Memory freeing function for use with option setting
 */
nag_opt_free(&options, "", &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(x);
NAG_FREE(hess);

```

```

NAG_FREE(ha);
NAG_FREE(ka);
NAG_FREE(hhess);
NAG_FREE(khess);
NAG_FREE(crnames);
NAG_FREE(names);

return exit_status;
}

static void NAG_CALL qp Hess (Integer ncolh, const double x[], double hx[],
                             Nag_Comm *comm)
{
  Integer      i, j, jrow;
  HessianData *hd = (HessianData *) (comm->p);
  double       *hess = hd->hess;
  Integer      *hhess = hd->hhess;
  Integer      *khess = hd->khess;

  for (i = 0; i < ncolh; ++i)
    hx[i] = 0.0;

  for (i = 0; i < ncolh; ++i)
  {
    /* For each column of Hessian */
    for (j = khess[i]; j < khess[i+1]; ++j)
    {
      /* For each non-zero in column */

      jrow = hhess[j] - 1;

      /* Using symmetry of hessian, add contribution
       * to hx of hess[j] as a diagonal or upper
       * triangular element of hessian.
       */
      hx[i] += hess[j]*x[jrow];

      /* If hess[j] not a diagonal element add its
       * contribution to hx as a lower triangular
       * element of hessian.
       */
      if (jrow != i)
        hx[jrow] += hess[j]*x[i];
    }
  }
} /* qp Hess */

```

## 10.2 Program Data

nag\_opt\_sparse\_convex\_qp (e04nkc) Example Program Data

Values of n and m

7 8

Values of nnz, iobj and ncolh

48 8 7

Matrix nonzeros: value, row index, column index

0.02	7	1
0.02	5	1
0.03	3	1
1.00	1	1
0.70	6	1
0.02	4	1
0.15	2	1
-200.00	8	1
0.06	7	2
0.75	6	2
0.03	5	2

```

0.04  4  2
0.05  3  2
0.04  2  2
1.00  1  2
-2000.00  8  2
0.02  2  3
1.00  1  3
0.01  4  3
0.08  3  3
0.08  7  3
0.80  6  3
-2000.00  8  3
1.00  1  4
0.12  7  4
0.02  3  4
0.02  4  4
0.75  6  4
0.04  2  4
-2000.00  8  4
0.01  5  5
0.80  6  5
0.02  7  5
1.00  1  5
0.02  2  5
0.06  3  5
0.02  4  5
-2000.00  8  5
1.00  1  6
0.01  2  6
0.01  3  6
0.97  6  6
0.01  7  6
400.00  8  6
0.97  7  7
0.03  2  7
1.00  1  7
400.00  8  7

```

Lower bounds

```

0.0      0.0      4.0e+02   1.0e+02   0.0      0.0      0.0      2.0e+03
-1.0e+25 -1.0e+25 -1.0e+25 -1.0e+25 1.5e+03 2.5e+02 -1.0e+25

```

Upper bounds

```

2.0e+02  2.5e+03  8.0e+02  7.0e+02  1.5e+03  1.0e+25  1.0e+25  2.0e+03
6.0e+01  1.0e+02  4.0e+01  3.0e+01  1.0e+25  3.0e+02  1.0e+25

```

Column and row names

```

'COLUMN 1' 'COLUMN 2' 'COLUMN 3' 'COLUMN 4' 'COLUMN 5' 'COLUMN 6' 'COLUMN 7'
'OBJECTIV' 'ROW    1' 'ROW    2' 'ROW    3' 'ROW    4' 'ROW    5' 'ROW    6'
'ROW      7'

```

Initial estimate of x

```

0.0 0.0 0.0 0.0 0.0 0.0 0.0

```

Number of hessian nonzeros

9

Hessian nonzeros: value, row index, col index (diagonal/lower triangle elements)

```

2.0 1 1
2.0 2 2
2.0 3 3
2.0 4 3
2.0 4 4
2.0 5 5
2.0 6 6
2.0 7 6
2.0 7 7

```

### 10.3 Program Results

nag\_opt\_sparse\_convex\_qp (e04nkc) Example Program Results

Parameters to e04nkc  
-----

```

Problem type..... sparse QP      Number of variables.....      7
Linear constraints.....          8      Hessian columns.....          7

prob_name.....
obj_name.....                    rhs_name.....
range_name.....                  bnd_name.....
crnames..... supplied

minimize..... Nag_TRUE          start..... Nag_Cold
ftol..... 1.00e-06             reset_ftol..... 10000
fcheck..... 60                 factor_freq..... 100
scale..... Nag_ExtraScale      scale_tol..... 9.00e-01
optim_tol..... 1.00e-06        max_iter..... 75
crash..... Nag_CrashTwice      crash_tol..... 1.00e-01
partial_price..... 10          pivot_tol..... 2.05e-11
max_sb..... 7
inf_bound..... 1.00e+20        inf_step..... 1.00e+20
lu_factor_tol..... 1.00e+02    lu_update_tol..... 1.00e+01
lu_sing_tol..... 2.05e-11      machine precision..... 1.11e-16
print_level..... Nag_Soln_Iter
outfile..... stdout
    
```

Memory allocation:  
state..... Nag lambda..... Nag

Itn	Step	Ninf	Sinf/Objective	Norm rg
Itn 0 -- Infeasible				
0	0.0e+00	1	1.152891e+03	0.0e+00
1	4.3e+02	0	0.000000e+00	0.0e+00
Itn 1 -- Feasible point found (for 1 equality constraints).				
1	0.0e+00	0	0.000000e+00	0.0e+00
1	0.0e+00	0	1.460000e+06	0.0e+00
Itn 1 -- Feasible QP solution.				
2	8.7e-02	0	9.409959e+05	0.0e+00
3	5.3e-01	0	-1.056552e+06	0.0e+00
4	1.0e+00	0	-1.462190e+06	4.1e-12
5	1.0e+00	0	-1.698092e+06	1.8e-12
6	4.6e-02	0	-1.764906e+06	7.0e+02
7	1.0e+00	0	-1.811946e+06	9.1e-13
8	1.7e-02	0	-1.847325e+06	1.7e+02
9	1.0e+00	0	-1.847785e+06	5.2e-12

Variable	State	Value	Lower Bound	Upper Bound	Lagr Mult	Residual
COLUMN 1	LL	0.00000e+00	0.0000e+00	2.0000e+02	2.361e+03	0.000e+00
COLUMN 2	BS	3.49399e+02	0.0000e+00	2.5000e+03	-1.062e-12	3.494e+02
COLUMN 3	SBS	6.48853e+02	4.0000e+02	8.0000e+02	-4.395e-12	1.511e+02
COLUMN 4	SBS	1.72847e+02	1.0000e+02	7.0000e+02	-2.274e-12	7.285e+01
COLUMN 5	BS	4.07521e+02	0.0000e+00	1.5000e+03	-2.067e-12	4.075e+02
COLUMN 6	BS	2.71356e+02	0.0000e+00	None	7.455e-13	2.714e+02
COLUMN 7	BS	1.50023e+02	0.0000e+00	None	4.710e-13	1.500e+02

Constrnt	State	Value	Lower Bound	Upper Bound	Lagr Mult	Residual
OBJECTIV	EQ	2.00000e+03	2.0000e+03	2.0000e+03	-1.290e+04	-0.000e+00
ROW 1	BS	4.92316e+01	None	6.0000e+01	-1.349e-11	-1.077e+01
ROW 2	UL	1.00000e+02	None	1.0000e+02	-2.325e+03	0.000e+00
ROW 3	BS	3.20719e+01	None	4.0000e+01	0.000e+00	-7.928e+00
ROW 4	BS	1.45572e+01	None	3.0000e+01	0.000e+00	-1.544e+01
ROW 5	LL	1.50000e+03	1.5000e+03	None	1.445e+04	-0.000e+00
ROW 6	LL	2.50000e+02	2.5000e+02	3.0000e+02	1.458e+04	-0.000e+00
ROW 7	BS	-2.98869e+06	None	None	-1.000e+00	-2.989e+06

Exit after 9 iterations.

Optimal QP solution found.

Final QP objective value = -1.8477847e+06

Perturb the problem and re-solve with warm start.

Parameters to e04nkc

```

-----
Problem type..... sparse QP      Number of variables..... 7
Linear constraints..... 8        Hessian columns..... 7

prob_name.....
obj_name.....          rhs_name.....
range_name.....       bnd_name.....
crnames..... supplied

minimize..... Nag_TRUE      start..... Nag_Warm
ftol..... 1.00e-06         reset_ftol..... 10000
fcheck..... 60            factor_freq..... 100
scale..... Nag_ExtraScale  scale_tol..... 9.00e-01
optim_tol..... 1.00e-06    max_iter..... 75
crash..... Nag_CrashTwice  crash_tol..... 1.00e-01
partial_price..... 10      pivot_tol..... 2.05e-11
max_sb..... 7
inf_bound..... 1.00e+20    inf_step..... 1.00e+20
lu_factor_tol..... 1.00e+02 lu_update_tol..... 1.00e+01
lu_sing_tol..... 2.05e-11  machine_precision..... 1.11e-16
print_level..... Nag_Soln
outfile..... stdout

```

Memory allocation:

```
state..... Nag lambda..... Nag
```

Variable	State	Value	Lower Bound	Upper Bound	Lagr Mult	Residual
COLUMN 1	LL	0.00000e+00	0.0000e+00	2.0000e+02	2.360e+03	0.000e+00
COLUMN 2	SBS	3.49529e+02	0.0000e+00	2.5000e+03	-1.769e-12	3.495e+02
COLUMN 3	BS	6.48762e+02	4.0000e+02	8.0000e+02	-7.644e-13	1.512e+02
COLUMN 4	SBS	1.72618e+02	1.0000e+02	7.0000e+02	-1.624e-12	7.262e+01
COLUMN 5	BS	4.07596e+02	0.0000e+00	1.5000e+03	-3.446e-13	4.076e+02
COLUMN 6	BS	2.71446e+02	0.0000e+00	None	-5.964e-13	2.714e+02
COLUMN 7	BS	1.50048e+02	0.0000e+00	None	7.850e-13	1.500e+02

Constrnt	State	Value	Lower Bound	Upper Bound	Lagr Mult	Residual
OBJECTIV	EQ	2.00000e+03	2.0000e+03	2.0000e+03	-1.290e+04	-0.000e+00
ROW 1	BS	4.92290e+01	None	6.0000e+01	0.000e+00	-1.077e+01
ROW 2	UL	1.00000e+02	None	1.0000e+02	-2.325e+03	0.000e+00
ROW 3	BS	3.20731e+01	None	4.0000e+01	0.000e+00	-7.927e+00
ROW 4	BS	1.45618e+01	None	3.0000e+01	0.000e+00	-1.544e+01
ROW 5	LL	1.50000e+03	1.5000e+03	None	1.446e+04	-0.000e+00
ROW 6	LL	2.50000e+02	2.5000e+02	3.0000e+02	1.458e+04	-0.000e+00
ROW 7	BS	-2.98841e+06	None	None	-1.000e+00	-2.988e+06

Exit after 1 iterations.

Optimal QP solution found.

Final QP objective value = -1.8466439e+06

## 11 Further Description

This section gives a detailed description of the algorithm used in `nag_opt_sparse_convex_qp` (e04nkc). 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

`nag_opt_sparse_convex_qp` (e04nkc) is based on an inertia-controlling method that maintains a Cholesky factorization of the reduced Hessian (see below). The method is similar to that of Gill and Murray (1978), and is described in detail by Gill *et al.* (1991). Here we briefly summarise the main features of the method. Where possible, explicit reference is made to the names of variables that are arguments of the function or appear in the printed output.

The method used has two distinct phases: finding an initial feasible point by minimizing the sum of infeasibilities (the *feasibility phase*), and minimizing the quadratic objective function within the feasible region (the *optimality phase*). The computations in both phases are performed by the same code. The two-phase nature of the algorithm is reflected by changing the function being minimized from the sum of infeasibilities (the quantity `Sinf` described in Section 5.1) to the quadratic objective function (the quantity `Objective`, see Section 5.1).

In general, an iterative process is required to solve a quadratic program. Given an iterate  $(x, s)$  in both the original variables  $x$  and the slack variables  $s$ , a new iterate  $(\bar{x}, \bar{s})$  is defined by

$$\begin{pmatrix} \bar{x} \\ \bar{s} \end{pmatrix} = \begin{pmatrix} x \\ s \end{pmatrix} + \alpha p, \quad (2)$$

where the *step length*  $\alpha$  is a non-negative scalar (the printed quantity `Step`, see Section 5.1), and  $p$  is called the *search direction*. (For simplicity, we shall consider a typical iteration and avoid reference to the index of the iteration.) Once an iterate is feasible (i.e., satisfies the constraints), all subsequent iterates remain feasible.

## 11.2 Definition of the Working Set and Search Direction

At each iterate  $(x, s)$ , a *working set* of constraints is defined to be a linearly independent subset of the constraints that are satisfied ‘exactly’ (to within the value of the optional argument `options.ftol`; see Section 12.2). The working set is the current prediction of the constraints that hold with equality at a solution of the LP or QP problem. Let  $m_W$  denote the number of constraints in the working set (including bounds), and let  $W$  denote the associated  $m_W$  by  $(n + m)$  *working set matrix* consisting of the  $m_W$  gradients of the working set constraints.

The search direction is defined so that constraints in the working set remain *unaltered* for any value of the step length. It follows that  $p$  must satisfy the identity

$$Wp = 0. \quad (3)$$

This characterisation allows  $p$  to be computed using any  $n$  by  $n_Z$  full-rank matrix  $Z$  that spans the null space of  $W$ . (Thus,  $n_Z = n - m_W$  and  $WZ = 0$ .) The null space matrix  $Z$  is defined from a sparse *LU* factorization of part of  $W$  (see (6) and (7) below). The direction  $p$  will satisfy (3) if

$$p = Zp_Z, \quad (4)$$

where  $p_Z$  is any  $n_Z$ -vector.

The working set contains the constraints  $Ax - s = 0$  and a subset of the upper and lower bounds on the variables  $(x, s)$ . Since the gradient of a bound constraint  $x_j \geq l_j$  or  $x_j \leq u_j$  is a vector of all zeros except for  $\pm 1$  in position  $j$ , it follows that the working set matrix contains the rows of  $(A \quad -I)$  and the unit rows associated with the upper and lower bounds in the working set.

The working set matrix  $W$  can be represented in terms of a certain column partition of the matrix  $(A \quad -I)$ . As in Section 3 we partition the constraints  $Ax - s = 0$  so that

$$Bx_B + Sx_S + Nx_N = 0, \quad (5)$$

where  $B$  is a square nonsingular basis and  $x_B$ ,  $x_S$  and  $x_N$  are the basic, superbasic and nonbasic variables respectively. The nonbasic variables are equal to their upper or lower bounds at  $(x, s)$ , and the superbasic variables are independent variables that are chosen to improve the value of the current objective function. The number of superbasic variables is  $n_S$  (the quantity `Ns` in the detailed printed output; see Section 12.3). Given values of  $x_N$  and  $x_S$ , the basic variables  $x_B$  are adjusted so that  $(x, s)$  satisfies (5).

If  $P$  is a permutation matrix such that  $(A \ -I)P = (B \ S \ N)$ , then the working set matrix  $W$  satisfies

$$WP = \begin{pmatrix} B & S & N \\ 0 & 0 & I_N \end{pmatrix}, \quad (6)$$

where  $I_N$  is the identity matrix with the same number of columns as  $N$ .

The null space matrix  $Z$  is defined from a sparse  $LU$  factorization of part of  $W$ . In particular,  $Z$  is maintained in ‘reduced gradient’ form, using the LUSOL package (see Gill *et al.* (1987)) to maintain sparse  $LU$  factors of the basis matrix  $B$  that alters as the working set  $W$  changes. Given the permutation  $P$ , the null space basis is given by

$$Z = P \begin{pmatrix} -B^{-1}S \\ I \\ 0 \end{pmatrix}. \quad (7)$$

This matrix is used only as an operator, i.e., it is never computed explicitly. Products of the form  $Zv$  and  $Z^Tg$  are obtained by solving with  $B$  or  $B^T$ . This choice of  $Z$  implies that  $n_Z$ , the number of ‘degrees of freedom’ at  $(x, s)$ , is the same as  $n_S$ , the number of superbasic variables.

Let  $g_Z$  and  $H_Z$  denote the *reduced gradient* and *reduced Hessian* of the objective function:

$$g_Z = Z^Tg \quad \text{and} \quad H_Z = Z^THZ, \quad (8)$$

where  $g$  is the objective gradient at  $(x, s)$ . Roughly speaking,  $g_Z$  and  $H_Z$  describe the first and second derivatives of an  $n_S$ -dimensional *unconstrained* problem for the calculation of  $p_Z$ . (The condition estimator of  $H_Z$  is the quantity  $\text{Cond } H_Z$  in the detailed printed output; see Section 12.3.)

At each iteration, an upper triangular factor  $R$  is available such that  $H_Z = R^TR$ . Normally,  $R$  is computed from  $R^TR = Z^THZ$  at the start of the optimality phase and then updated as the QP working set changes. For efficiency, the dimension of  $R$  should not be excessive (say,  $n_S \leq 1000$ ). This is guaranteed if the number of nonlinear variables is ‘moderate’.

If the QP problem contains linear variables,  $H$  is positive semidefinite and  $R$  may be singular with at least one zero diagonal element. However, an inertia-controlling strategy is used to ensure that only the last diagonal element of  $R$  can be zero. (See Gill *et al.* (1991) for a discussion of a similar strategy for indefinite quadratic programming.)

If the initial  $R$  is singular, enough variables are fixed at their current value to give a nonsingular  $R$ . This is equivalent to including temporary bound constraints in the working set. Thereafter,  $R$  can become singular only when a constraint is deleted from the working set (in which case no further constraints are deleted until  $R$  becomes nonsingular).

### 11.3 The Main Iteration

If the reduced gradient is zero,  $(x, s)$  is a constrained stationary point on the working set. During the feasibility phase, the reduced gradient will usually be zero only at a vertex (although it may be zero elsewhere in the presence of constraint dependencies). During the optimality phase, a zero reduced gradient implies that  $x$  minimizes the quadratic objective function when the constraints in the working set are treated as equalities. At a constrained stationary point, Lagrange multipliers  $\lambda$  are defined from the equations

$$W^T\lambda = g(x). \quad (9)$$

A Lagrange multiplier  $\lambda_j$  corresponding to an inequality constraint in the working set is said to be *optimal* if  $\lambda_j \leq \sigma$  when the associated constraint is at its *upper bound*, or if  $\lambda_j \geq -\sigma$  when the associated constraint is at its *lower bound*, where  $\sigma$  depends on the value of the optional argument **options.optim\_tol** (see Section 12.2). If a multiplier is non-optimal, the objective function (either the true objective or the sum of infeasibilities) can be reduced by continuing the minimization with the corresponding constraint excluded from the working set. (This step is sometimes referred to as ‘deleting’ a constraint from the working set.) If optimal multipliers occur during the feasibility phase but the sum of infeasibilities is nonzero, there is no feasible point and the function terminates immediately with **fail.code** = NW\_NOT\_FEASIBLE (see Section 6).

The special form (6) of the working set allows the multiplier vector  $\lambda$ , the solution of (9), to be written in terms of the vector

$$d = \begin{pmatrix} g \\ 0 \end{pmatrix} - (A \quad -I)^T \pi = \begin{pmatrix} g - A^T \pi \\ \pi \end{pmatrix}, \quad (10)$$

where  $\pi$  satisfies the equations  $B^T \pi = g_B$ , and  $g_B$  denotes the basic elements of  $g$ . The elements of  $\pi$  are the Lagrange multipliers  $\lambda_j$  associated with the equality constraints  $Ax - s = 0$ . The vector  $d_N$  of nonbasic elements of  $d$  consists of the Lagrange multipliers  $\lambda_j$  associated with the upper and lower bound constraints in the working set. The vector  $d_S$  of superbasic elements of  $d$  is the reduced gradient  $g_Z$  in (8). The vector  $d_B$  of basic elements of  $d$  is zero, by construction. (The Euclidean norm of  $d_S$  and the final values of  $d_S$ ,  $g$  and  $\pi$  are the quantities Norm rg, Reduced Gradnt, Obj Gradient and Dual Activity in the detailed printed output; see Section 12.3.)

If the reduced gradient is not zero, Lagrange multipliers need not be computed and the search direction is given by  $p = Zp_Z$  (see (7) and (11)). The step length is chosen to maintain feasibility with respect to the satisfied constraints.

There are two possible choices for  $p_Z$ , depending on whether or not  $H_Z$  is singular. If  $H_Z$  is nonsingular,  $R$  is nonsingular and  $p_Z$  in (4) is computed from the equations

$$R^T R p_Z = -g_Z, \quad (11)$$

where  $g_Z$  is the reduced gradient at  $x$ . In this case,  $(x, s) + p$  is the minimizer of the objective function subject to the working set constraints being treated as equalities. If  $(x, s) + p$  is feasible,  $\alpha$  is defined to be unity. In this case, the reduced gradient at  $(\bar{x}, \bar{s})$  will be zero, and Lagrange multipliers are computed at the next iteration. Otherwise,  $\alpha$  is set to  $\alpha_M$ , the step to the ‘nearest’ constraint along  $p$ . This constraint is added to the working set at the next iteration.

If  $H_Z$  is singular, then  $R$  must also be singular, and an inertia-controlling strategy is used to ensure that only the last diagonal element of  $R$  is zero. (See Gill *et al.* (1991) for a discussion of a similar strategy for indefinite quadratic programming.) In this case,  $p_Z$  satisfies

$$p_Z^T H_Z p_Z = 0 \quad \text{and} \quad g_Z^T p_Z \leq 0, \quad (12)$$

which allows the objective function to be reduced by any step of the form  $(x, s) + \alpha p$ , where  $\alpha > 0$ . The vector  $p = Zp_Z$  is a direction of unbounded descent for the QP problem in the sense that the QP objective is linear and decreases without bound along  $p$ . If no finite step of the form  $(x, s) + \alpha p$  (where  $\alpha > 0$ ) reaches a constraint not in the working set, the QP problem is unbounded and the function terminates immediately with **fail.code** = NE\_UNBOUNDED (see Section 6). Otherwise,  $\alpha$  is defined as the maximum feasible step along  $p$  and a constraint active at  $(x, s) + \alpha p$  is added to the working set for the next iteration.

#### 11.4 Miscellaneous

If the basis matrix is not chosen carefully, the condition of the null space matrix  $Z$  in (7) could be arbitrarily high. To guard against this, the function implements a ‘basis repair’ feature in which the LUSOL package (see Gill *et al.* (1987)) is used to compute the rectangular factorization

$$(B \quad S)^T = LU, \quad (13)$$

returning just the permutation  $P$  that makes  $PLP^T$  unit lower triangular. The pivot tolerance is set to require  $|PLP^T|_{ij} \leq 2$ , and the permutation is used to define  $P$  in (6). It can be shown that  $\|Z\|$  is likely to be little more than unity. Hence,  $Z$  should be well conditioned *regardless of the condition of  $W$* . This feature is applied at the beginning of the optimality phase if a potential  $B - S$  ordering is known.

The EXPAND procedure (see Gill *et al.* (1989)) is used to reduce the possibility of cycling at a point where the active constraints are nearly linearly dependent. Although there is no absolute guarantee that cycling will not occur, the probability of cycling is extremely small (see Hall and McKinnon (1996)). The main feature of EXPAND is that the feasibility tolerance is increased at the start of every iteration. This allows a positive step to be taken at every iteration, perhaps at the expense of violating the bounds on  $(x, s)$  by a small amount.



Suppose that the value of the optional argument **options.ftol** (see Section 12.2) is  $\delta$ . Over a period of  $K$  iterations (where  $K$  is the value of the optional argument **options.reset\_ftol**; see Section 12.2), the feasibility tolerance actually used by `nag_opt_sparse_convex_qp` (e04nkc) (i.e., the *working* feasibility tolerance) increases from  $0.5\delta$  to  $\delta$  (in steps of  $0.5\delta/K$ ).

At certain stages the following ‘resetting procedure’ is used to remove small constraint infeasibilities. First, all nonbasic variables are moved exactly onto their bounds. A count is kept of the number of non-trivial adjustments made. If the count is nonzero, the basic variables are recomputed. Finally, the working feasibility tolerance is reinitialized to  $0.5\delta$ .

If a problem requires more than  $K$  iterations, the resetting procedure is invoked and a new cycle of iterations is started. (The decision to resume the feasibility phase or optimality phase is based on comparing any constraint infeasibilities with  $\delta$ .)

The resetting procedure is also invoked when `nag_opt_sparse_convex_qp` (e04nkc) reaches an apparently optimal, infeasible or unbounded solution, unless this situation has already occurred twice. If any non-trivial adjustments are made, iterations are continued.

The EXPAND procedure not only allows a positive step to be taken at every iteration, but also provides a potential *choice* of constraints to be added to the working set. All constraints at a distance  $\alpha$  (where  $\alpha \leq \alpha_M$ ) along  $p$  from the current point are then viewed as acceptable candidates for inclusion in the working set. The constraint whose normal makes the largest angle with the search direction is added to the working set. This strategy helps keep the basis matrix  $B$  well conditioned.

## 12 Optional Arguments

A number of optional input and output arguments to `nag_opt_sparse_convex_qp` (e04nkc) 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_sparse_convex_qp` (e04nkc); 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 **not** be preceded by initialization.

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

### 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_sparse_convex_qp` (e04nkc) 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>
<code>Nag_PrintType</code> print_level	<b><code>Nag_Soln_Iter</code></b>
char outfile[80]	stdout
void (*print_fun)()	<b>NULL</b>
char prob_name[9]	'\0'
char obj_name[9]	'\0'
char rhs_name[9]	'\0'
char range_name[9]	'\0'

char bnd_name[9]	'\0'
char **crnames	NULL
Boolean minimize	Nag_TRUE
Integer max_iter	max(50, 5(n + m))
Nag_CrashType crash	Nag_CrashTwice
double crash_tol	0.1
Nag_ScaleType scale	Nag_ExtraScale
double scale_tol	0.9
double optim_tol	max( $10^{-6}$ , $\sqrt{\epsilon}$ )
double ftol	max( $10^{-6}$ , $\sqrt{\epsilon}$ )
Integer reset_ftol	10000
Integer fcheck	60
Integer factor_freq	100
Integer partial_price	10
double pivot_tol	$\epsilon^{0.67}$
double lu_factor_tol	100.0
double lu_update_tol	10.0
double lu_sing_tol	$\epsilon^{0.67}$
Integer max_sb	min(ncolh + 1n)
double inf_bound	$10^{20}$
double inf_step	max(options.inf_bound, $10^{20}$ )
Integer *state	size n + m
double *lambda	size n + m
Integer nsb	
Integer iter	
Integer nf	

## 12.2 Description of the Optional Arguments

**start** – Nag\_Start Default = Nag\_Cold

*On entry:* specifies how the initial working set is to be chosen.

**options.start** = Nag\_Cold

An internal Crash procedure will be used to choose an initial basis matrix,  $B$ .

**options.start** = Nag\_Warm

You must provide a valid definition of every array element of the optional argument **options.state** (see below), probably obtained from a previous call of `nag_opt_sparse_convex_qp` (e04nkc), while, for QP problems, the optional argument **options.nsb** (see below) must retain its value from a previous call.

*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_sparse_convex_qp` (e04nkc) will be printed.

**print\_level** – Nag\_PrintType Default = Nag\_Soln\_Iter

*On entry:* the level of results printout produced by nag\_opt\_sparse\_convex\_qp (e04nkc). The following values are available:

Nag_NoPrint	No output.
Nag_Soln	The final solution.
Nag_Iter	One line of output for each iteration.
Nag_Iter_Long	A longer line of output for each iteration with more information (line exceeds 80 characters).
Nag_Soln_Iter	The final solution and one line of output for each iteration.
Nag_Soln_Iter_Long	The final solution and one long line of output for each iteration (line exceeds 80 characters).
Nag_Soln_Iter_Full	As Nag_Soln_Iter_Long with the matrix statistics (initial status of rows and columns, number of elements, density, biggest and smallest elements, etc.), factors resulting from the scaling procedure (if <b>options.scale</b> = Nag_RowColScale or Nag_ExtraScale; see below), basis factorization statistics and details of the initial basis resulting from the Crash procedure (if <b>options.start</b> = Nag_Cold).

Details of each level of results printout are described in Section 12.3.

*Constraint:* **options.print\_level** = Nag\_NoPrint, Nag\_Soln, Nag\_Iter, Nag\_Soln\_Iter, Nag\_Iter\_Long, Nag\_Soln\_Iter\_Long or Nag\_Soln\_Iter\_Full.

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

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

**print\_fun** – pointer to function Default = NULL

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

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

See Section 12.3.1 below for further details.

<b>prob_name</b> – const char	Default: <b>options.prob_name</b> [0] = '\0'
<b>obj_name</b> – const char	Default: <b>options.obj_name</b> [0] = '\0'
<b>rhs_name</b> – const char	Default: <b>options.rhs_name</b> [0] = '\0'
<b>range_name</b> – const char	Default: <b>options.range_name</b> [0] = '\0'
<b>bnd_name</b> – const char	Default: <b>options.bnd_name</b> [0] = '\0'

*On entry:* these options contain the names associated with the so-called MPSX form of the problem. The arguments contain, respectively, the names of: the problem; the objective (or free) row; the constraint right-hand side; the ranges, and the bounds. They are used in the detailed output when optional argument **options.print\_level** = Nag\_Soln\_Iter\_Full.

**crnames** – char \*\* Default = NULL

*On entry:* if **options.crnames** is not NULL then it must point to an array of  $n + m$  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  $j = 1, 2, \dots, n$ , and **options.crnames**[ $n + i - 1$ ] contains the names of the  $i$ th row (constraint), for  $i = 1, 2, \dots, m$ . If supplied, the names are used in the solution output (see Section 5.1 and Section 12.3).

**minimize** – Nag\_Boolean Default = Nag\_TRUE

*On entry:* **options.minimize** specifies the required 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  $d_j$  (see Section 11.3) will be reversed.

**max\_iter** – Integer Default =  $\max(50, 5(\mathbf{n} + \mathbf{m}))$

*On entry:* **options.max\_iter** specifies the maximum number of iterations allowed before termination.

If you wish to check that a call to `nag_opt_sparse_convex_qp` (e04nkc) is correct before attempting to solve the problem in full then **options.max\_iter** may be set to 0. No iterations will then be performed but all initialization prior to the first iteration will be done and a listing of argument settings will be output, if optional argument **options.list** = Nag\_TRUE (the default setting).

*Constraint:* **options.max\_iter**  $\geq 0$ .

**crash** – Nag\_CrashType Default = Nag\_CrashTwice

This option does not apply when optional argument **options.start** = Nag\_Warm.

*On entry:* if **options.start** = Nag\_Cold, and internal Crash procedure is used to select an initial basis from various rows and columns of the constraint matrix  $(A \ -I)$ . The value of **options.crash** determines which rows and columns are initially eligible for the basis, and how many times the Crash procedure is called.

If **options.crash** = Nag\_NoCrash, the all-slack basis  $B = -I$  is chosen.

**options.crash** = Nag\_CrashOnce

The Crash procedure is called once (looking for a triangular basis in all rows and columns of the linear constraint matrix  $A$ ).

**options.crash** = Nag\_CrashTwice

The Crash procedure is called twice (looking at any *equality* constraints first followed by any *inequality* constraints).

If **options.crash** = Nag\_CrashOnce or Nag\_CrashTwice, certain slacks on inequality rows are selected for the basis first. (If **options.crash** = Nag\_CrashTwice, 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 or Nag\_CrashTwice.

**crash\_tol** – double Default = 0.1

*On entry:* **options.crash\_tol** allows the Crash procedure to ignore certain ‘small’ nonzero elements in the constraint matrix  $A$  while searching for a triangular basis. For each column of  $A$ , if  $a_{\max}$  is the largest element in the column, other nonzeros in that column are ignored if they are less than (or equal to)  $a_{\max} \times$  **options.crash\_tol**.

When **options.crash\_tol**  $> 0$ , the basis obtained by the Crash procedure may not be strictly triangular, but it is likely to be nonsingular and almost triangular. The intention is to obtain a starting basis with more column variables and fewer (arbitrary) slacks. A feasible solution may be reached earlier for some problems.

*Constraint:*  $0.0 \leq$  **options.crash\_tol**  $< 1.0$ .

**scale** – Nag\_ScaleType Default = Nag\_ExtraScale

*On entry:* this option enables the scaling of 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. This may improve the overall

efficiency of the function on some problems. (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  $j > n$ .)

**options.scale** = Nag\_NoScale

No scaling is performed.

**options.scale** = Nag\_RowColScale

All rows and columns of the constraint matrix  $A$  are scaled.

**options.scale** = Nag\_ExtraScale

An additional scaling is performed that may be helpful when the solution  $x$  is large; it takes into account columns of  $(A \ -I)$  that are fixed or have positive lower bounds or negative upper bounds.

*Constraint:* **options.scale** = Nag\_NoScale, Nag\_RowColScale or Nag\_ExtraScale.

**scale\_tol** – double

Default = 0.9

This option does not apply when optional argument **options.scale** = Nag\_NoScale.

*On entry:* **options.scale\_tol** 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., ('biggest' element)/('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:*  $0.0 < \mathbf{options.scale\_tol} < 1.0$ .

**optim\_tol** – double

Default =  $\max(10^{-6}, \sqrt{\epsilon})$

*On entry:* **options.optim\_tol** is used to judge the size of the reduced gradients  $d_j = g_j - \pi^T a_j$ . By definition, the reduced gradients for basic variables are always zero. Optimality is declared if the reduced gradients for any nonbasic variables at their lower or upper bounds satisfy  $-\mathbf{options.optim\_tol} \times \max(1, |\pi|) \leq d_j \leq \mathbf{options.optim\_tol} \times \max(1, |\pi|)$ , and if  $|d_j| \leq \mathbf{options.optim\_tol} \times \max(1, |\pi|)$  for any superbasic variables.

*Constraint:* **options.optim\_tol**  $\geq \epsilon$ .

**ftol** – double

Default =  $\max(10^{-6}, \sqrt{\epsilon})$

*On entry:* **options.ftol** defines the maximum acceptable *absolute* violation in each constraint at a 'feasible' point (including slack variables). For example, if the variables and the coefficients in the linear constraints are of order unity, and the latter are correct to about 6 decimal digits, it would be appropriate to specify **options.ftol** as  $10^{-6}$ .

nag\_opt\_sparse\_convex\_qp (e04nkc) attempts to find a feasible solution before optimizing the objective function. If the sum of infeasibilities cannot be reduced to zero, the problem is assumed to be *infeasible*. Let  $\text{Sinf}$  be the corresponding sum of infeasibilities. If  $\text{Sinf}$  is quite small, it may be appropriate to raise **options.ftol** by a factor of 10 or 100. Otherwise, some error in the data should be suspected. Note that nag\_opt\_sparse\_convex\_qp (e04nkc) does *not* attempt to find the minimum value of  $\text{Sinf}$ .

If the constraints and variables have been scaled (see optional argument **options.scale** above), then feasibility is defined in terms of the scaled problem (since it is more likely to be meaningful).

*Constraint:* **options.ftol**  $\geq \epsilon$ .

**reset\_ftol** – Integer

Default = 5

*On entry:* this option is part of an anti-cycling procedure designed to guarantee progress even on highly degenerate problems (see Section 11.4).

For LP problems, 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 the optional argument **options.ftol** is  $\delta$ . Over a period of **options.reset\_ftol** iterations, the feasibility tolerance actually used by

nag\_opt\_sparse\_convex\_qp (e04nkc) (i.e., the *working* feasibility tolerance) increases from  $0.5\delta$  to  $\delta$  (in steps of  $0.5\delta/\mathbf{options.reset\_ftol}$ ).

For QP problems, 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.reset\_ftol** 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).

*Constraint:*  $0 < \mathbf{options.reset\_ftol} < 10000000$ .

**fcheck** – Integer

Default = 60

*On entry:* every **options.fcheck**th iteration after the most recent basis factorization, a numerical test is made to see if the current solution  $(x, s)$  satisfies the linear constraints  $Ax - s = 0$ . If the largest element of the residual vector  $r = Ax - s$  is judged to be too large, the current basis is refactorized and the basic variables recomputed to satisfy the constraints more accurately.

*Constraint:* **options.fcheck**  $\geq 1$ .

**factor\_freq** – Integer

Default = 100

*On entry:* at most **options.factor\_freq** basis changes will occur between factorizations of the basis matrix. For LP problems, the basis factors are usually updated at every iteration. For QP problems, 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 optional argument **options.fcheck** to ensure that the linear constraints  $Ax - s = 0$  are satisfied. If necessary, the basis will be refactorized before the limit of **options.factor\_freq** updates is reached.

*Constraint:* **options.factor\_freq**  $\geq 1$ .

**partial\_price** – Integer

Default = 10

This option does not apply to QP problems.

*On entry:* this option is recommended for large FP or LP problems that have significantly more variables than constraints (i.e.,  $n \gg m$ ). It reduces the work required for each pricing operation (i.e., when a nonbasic variable is selected to enter the basis). If **options.partial\_price** = 1, all columns of the constraint matrix  $(A \ -I)$  are searched. If **options.partial\_price**  $> 1$ ,  $A$  and  $-I$  are partitioned to give **options.partial\_price** roughly equal segments  $A_j, K_j$ , for  $j = 1, 2, \dots, p$  (modulo  $p$ ). If the previous pricing search was successful on  $A_{j-1}, K_{j-1}$ , the next search begins on the segments  $A_j, K_j$ . 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  $A_{j+1}, K_{j+1}$ , and so on.

*Constraint:* **options.partial\_price**  $\geq 1$ .

**pivot\_tol** – double

Default =  $\epsilon^{0.67}$

*On entry:* **options.pivot\_tol** is used to prevent columns entering the basis if they would cause the basis to become almost singular.

*Constraint:* **options.pivot\_tol**  $> 0.0$ .

**lu\_factor\_tol** – double

Default = 100.0

**lu\_update\_tol** – double

Default = 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 lower triangular matrix  $L$  is a product of matrices of the form

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

where the multipliers  $\mu$  will satisfy  $|\mu| < \mathbf{options.lu\_factor\_tol}$  during refactorization or  $|\mu| < \mathbf{options.lu\_update\_tol}$  during update. The default values of **options.lu\_factor\_tol** and **options.lu\_update\_tol** usually strike a good compromise between stability and sparsity. For large and relatively dense problems, setting **options.lu\_factor\_tol** and **options.lu\_update\_tol** to 25 (say) may give a marked improvement in sparsity without impairing stability to a serious degree. Note that for band matrices it may be necessary to set **options.lu\_factor\_tol** in the range  $1 \leq \mathbf{options.lu\_factor\_tol} < 2$  in order to achieve stability.

*Constraints:*

**options.lu\_factor\_tol**  $\geq 1.0$ ;  
**options.lu\_update\_tol**  $\geq 1.0$ .

**lu\_sing\_tol** – double Default =  $\epsilon^{0.67}$

*On entry:* **options.lu\_sing\_tol** 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  $|u_{jj}| \leq \mathbf{options.lu\_sing\_tol}$  or  $|u_{jj}| < \mathbf{options.lu\_sing\_tol} \times \max_i |u_{ij}|$ , the  $j$ th column of the basis is replaced by the corresponding slack variable.

*Constraint:* **options.lu\_sing\_tol**  $> 0.0$ .

**max\_sb** – Integer Default =  $\min(\mathbf{ncolh} + 1, \mathbf{n})$

This option does not apply to FP or LP problems.

*On entry:* **options.max\_sb** places an upper bound on the number of variables which may enter the set of superbasic variables (see Section 11.2). If the number of superbasics exceeds this bound then nag\_opt\_sparse\_convex\_qp (e04nkc) will terminate with **fail.code** = NE\_HESS\_TOO\_BIG. In effect, **options.max\_sb** specifies ‘how nonlinear’ the QP problem is expected to be.

*Constraint:* **options.max\_sb**  $> 0$ .

**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  $-\mathbf{options.inf\_bound}$  will be regarded as  $-\infty$ ).

*Constraint:* **options.inf\_bound**  $> 0.0$ .

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

*On entry:* **options.inf\_step** specifies the magnitude of the change in variables that will be considered a step to an unbounded solution. (Note that an unbounded solution can occur only when the Hessian is not positive definite.) If the change in  $x$  during an iteration would exceed the value of **options.inf\_step**, the objective function is considered to be unbounded below in the feasible region.

*Constraint:* **options.inf\_step**  $> 0.0$ .

**state** – Integer \* Default memory =  $\mathbf{n} + \mathbf{m}$

*On entry:* **options.state** need not be set if the default option of **options.start** = Nag\_Cold is used as  $\mathbf{n} + \mathbf{m}$  values of memory will be automatically allocated by nag\_opt\_sparse\_convex\_qp (e04nkc).

If the option **options.start** = Nag\_Warm has been chosen, **options.state** must point to a minimum of  $\mathbf{n} + \mathbf{m}$  elements of memory. This memory will already be available if the **options** structure has been used in a previous call to nag\_opt\_sparse\_convex\_qp (e04nkc) from the calling program, with **options.start** = Nag\_Cold and the same values of  $\mathbf{n}$  and  $\mathbf{m}$ . 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  $j = 1, 2, \dots, n$ , are:

<b>options.state</b> $[j]$	State of <b>xs</b> $[j]$ 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** $[j] = 0$  (and **xs** $[j] = 0.0$ ), for  $j = 0, 1, \dots, n - 1$ . 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** $[j] = 4$  and **xs** $[j] = \mathbf{bl}[j]$  or **options.state** $[j] = 5$  and **xs** $[j] = \mathbf{bu}[j]$  as appropriate.

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

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\_sparse\_convex\_qp (e04nkc) has been called previously with the same values of **n** and **m**, **options.state** already contains satisfactory information.

*Constraints:*

$$0 \leq \mathbf{options.state}[j] \leq 5 \text{ if } \mathbf{options.start} = \text{Nag\_Cold, for } j = 0, 1, \dots, n - 1;$$

$$0 \leq \mathbf{options.state}[j] \leq 3 \text{ if } \mathbf{options.start} = \text{Nag\_Warm, for } j = 0, 1, \dots, n + m - 1.$$

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

If the problem is feasible (i.e., **ninf** = 0), basic and superbasic variables may be outside their bounds by as much as optional argument **options.ftol**. Note that unless the optional argument **options.scale** = Nag\_NoScale, **options.ftol** 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.ftol**, and there may be some nonbasic variables for which **xs** $[j]$  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 **options.scale** = Nag\_NoScale).

**lambda** – double \*

Default memory = **n + m**

*On entry:* **n + m** values of memory will be automatically allocated by nag\_opt\_sparse\_convex\_qp (e04nkc) and this is the recommended method of use of **options.lambda**. However you may supply memory from the calling program.

*On exit:* the values of the multipliers for each constraint with respect to the current working set. The first **n** elements contain the multipliers (*reduced costs*) for the bound constraints on the variables, and the next **m** elements contain the Lagrange multipliers (*shadow prices*) for the general linear constraints.



**nsb** – Integer

*On entry:*  $n_S$ , the number of superbasics. For QP problems, **options.nsb** need not be specified if optional argument **options.start** = Nag\_Cold, but must retain its value from a previous call when **options.start** = Nag\_Warm. For FP and LP problems, **options.nsb** is not referenced.

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

*On exit:* the final number of superbasics. This will be zero for FP and LP problems.

**iter** – Integer

*On exit:* the total number of iterations performed.

**nf** – Integer

*On exit:* the number of times the product  $Hx$  has been calculated (i.e., number of calls of **qphx**).

### 12.3 Description of Printed Output

The level of printed output can be controlled with the structure members **options.list** and **options.print\_level** (see Section 12.2). If **options.list** = Nag\_TRUE then the argument values to nag\_opt\_sparse\_convex\_qp (e04nkc) are listed, whereas the printout of results is governed by the value of **options.print\_level**. The default of **options.print\_level** = Nag\_Soln\_Iter provides a single short line of output at each iteration and the final result. This section describes all of the possible levels of results printout available from nag\_opt\_sparse\_convex\_qp (e04nkc).

When **options.print\_level** = Nag\_Iter or Nag\_Soln\_Iter the output produced at each iteration is as described in Section 5.1. If **options.print\_level** = Nag\_Iter\_Long, Nag\_Soln\_Iter\_Long or Nag\_Soln\_Iter\_Full the following, more detailed, line of output is produced at every iteration. In all cases, the values of the quantities printed are those in effect *on completion* of the given iteration.

Itn	is the iteration count.
pp	is the partial price indicator. The variable selected by the last pricing operation came from the ppth 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.
+S	is the variable selected by the pricing operation to be added to the superbasic set.
-S	is the variable chosen to leave the superbasic set.
-B	is the variable removed from the basis (if any) to become nonbasic.
-B	is the variable chosen to leave the set of basics (if any) in a special basic $\leftrightarrow$ superbasic swap. The entry under -S has become basic if this entry is nonzero, and nonbasic otherwise. The swap is done to ensure that there are no superbasic slacks.
Step	is the value of the steplength $\alpha$ taken along the computed search direction $p$ . The variables $x$ have been changed to $x + \alpha p$ . If a variable is made superbasic during the current iteration (i.e., +S 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 = $\epsilon^{0.67}$ , where $\epsilon$ is the <i>machine precision</i> ; see Section 12.2) to exclude very small elements of $y$ from consideration during the computation of Step.
Ninf	is the number of violated constraints (infeasibilities). This will be zero during the optimality phase.

Sinf/Objective	is the current value of the objective function. If $x$ is not feasible, Sinf gives the sum of magnitudes of constraint violations. If $x$ is feasible, Objective is the value of the objective function. The output line for the final iteration of the feasibility phase (i.e., the first iteration for which Ninf is zero) will give the value of the true objective at the first feasible point.  During the optimality phase, the value of the objective function will be non-increasing. During the feasibility phase, the number of constraint infeasibilities will not increase until either a feasible point is found, or the optimality of the multipliers implies that no feasible point exists.
L	is the number of nonzeros in the basis factor $L$ . Immediately after a basis factorization $B = LU$ , this is lenL, the number of subdiagonal elements in the columns of a lower triangular matrix. 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, this is lenU, the number of diagonal and superdiagonal elements in the rows of an upper triangular matrix. 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_sparse_convex_qp (e04nkc) will attempt to expand the internal workspace allocated for the basis factors.
Norm rg	is $\ d_S\ $ , the Euclidean norm of the reduced gradient (see Section 11.3). During the optimality phase, this norm will be approximately zero after a unit step. For FP and LP problems, Norm rg is not printed.
Ns	is the current number of superbasic variables. For FP and LP problems, Ns is not printed.
Cond Hz	is a lower bound on the condition number of the reduced Hessian (see Section 11.2). The larger this number, the more difficult the problem. For FP and LP problems, Cond Hz is not printed.

When **options.print\_level** = Nag\_Soln\_Iter\_Full the following intermediate printout (< 120 characters) is produced whenever the matrix  $B$  or  $B_S = (B \ S)^T$  is factorized. Gaussian elimination is used to compute an  $LU$  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** (see Section 12.2).

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	Number of updates reached the value of the optional argument <b>options.factor_freq</b> (see Section 12.2).
2	Excessive nonzeros in updated factors.
7	Not enough storage to update factors.
10	Row residuals too large (see the description for the optional argument <b>options.fcheck</b> in Section 12.2).
11	Ill conditioning has caused inconsistent results.

Iteration is the iteration count.

Nonlinear is the number of nonlinear variables in  $B$  (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.
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 $L$ (not printed if $B_S$ is factorized). This will not exceed the value of the optional argument <b>options.lu_factor_tol</b> .
$B_{\max}$	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 optional argument <b>options.lu_factor_tol</b> to a value near 1.0. $U_{\max}$ is not printed if $B_S$ is factorized.
$U_{\min}$	is the magnitude of the smallest diagonal element of $PUQ$ (not printed if $B_S$ is factorized).
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 could occur in subsequent computations. (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 refactorized.)  Growth is not printed if $B_S$ is factorized.
$L_t$	is the number of triangular columns of $B$ at the beginning of $L$ .
$\text{bp}$	is the size of the ‘bump’ or block to be factorized nontrivially after the triangular rows and columns have been removed.

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

When **options.print\_level** = Nag\_Soln\_Iter\_Full the following lines of intermediate printout (< 80 characters) are produced whenever **options.start** = Nag\_Cold (see Section 12.2). They refer to the number of columns selected by the Crash procedure during each of several passes through  $A$ , whilst 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.  
 Preferred is the number of 'preferred' columns in the basis (i.e., **options.state**[ $j$ ] = 3 for some  $j < n$ ).  
 Unit is the number of unit columns in the basis.  
 Double is the number of double columns in the basis.  
 Triangle is the number of triangular columns in the basis.  
 Pad is the number of slacks used to pad the basis.

When **options.print\_level** = Nag\_Soln\_Iter\_Full the following lines of intermediate printout (< 80 characters) are produced, following the final iteration. They refer to the 'MPSX names' stored in the optional arguments **options.prob\_name**, **options.obj\_name**, **options.rhs\_name**, **options.range\_name** and **options.bnd\_name** (see Section 12.2).

Name gives the name for the problem (blank if none).  
 Status gives the exit status for the problem (i.e., Optimal soln, Weak soln, Unbounded, Infeasible, Excess itns, Error condn or Feasble soln) followed by details of the direction of the optimization (i.e., (Min) or (Max)).  
 Objective gives the name of the free row for the problem (blank if none).  
 RHS gives the name of the constraint right-hand side for the problem (blank if none).  
 Ranges gives the name of the ranges for the problem (blank if none).  
 Bounds gives the name of the bounds for the problem (blank if none).

When **options.print\_level** = Nag\_Soln or Nag\_Soln\_Iter the final solution printout for each column and row is as described in Section 5.1. When **options.print\_level** = Nag\_Soln\_Iter\_Long or Nag\_Soln\_Iter\_Full, the following longer lines of final printout (< 120 characters) are produced.

Let  $a_j$  denote the  $j$ th column of  $A$ , for  $j = 1, 2, \dots, n$ . 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  $x_j$  (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  $x_j$ . Note that unless the optional argument **options.scale** = Nag\_NoScale (default value is **options.scale** = Nag\_ExtraScale; see Section 12.2) 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 bound, 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. However, if there are any degenerate variables (labelled D), the actual change might prove to be zero, since one of them could

encounter a bound immediately. In either case, the values of the Lagrange multipliers *might* also change.

- D *Degenerate.*  $x_j$  is basic or superbasic, but it is equal to (or very close to) one of its bounds.
- I *Infeasible.*  $x_j$  is basic or superbasic and is currently violating one of its bounds by more than the value of the optional argument **options.ftol** (default value =  $\max(10^{-6}, \sqrt{\epsilon})$ , where  $\epsilon$  is the *machine precision*; see Section 12.2).
- N *Not precisely optimal.*  $x_j$  is nonbasic or superbasic. If the value of the reduced gradient for  $x_j$  exceeds the value of the optional argument **options.optim\_tol** (default value =  $\max(10^{-6}, \sqrt{\epsilon})$ ; see Section 12.2), the solution would not be declared optimal because the reduced gradient for  $x_j$  would not be considered negligible.

Activity	is the value of $x_j$ at the final iterate.
Obj Gradient	is the value of $g_j$ at the final iterate. For FP problems, $g_j$ is set to zero.
Lower Bound	is the lower bound specified for $x_j$ . (None indicates that $\mathbf{bl}[j-1] \leq -\mathbf{options.inf\_bound}$ , where <b>options.inf_bound</b> is the optional argument.)
Upper Bound	is the upper bound specified for $x_j$ . (None indicates that $\mathbf{bu}[j-1] \geq \mathbf{options.inf\_bound}$ .)
Reduced Gradient	is the value of $d_j$ at the final iterate (see Section 11.3). For FP problems, $d_j$ is set to zero.
$m + j$	is the value of $m + j$ .
Let $v_i$ denote the $i$ th row of $A$ , for $i = 1, 2, \dots, m$ . 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 $v_i$ .
State	gives the state of $v_i$ (LL if active on its lower bound, UL if active on its upper bound, EQ if active and fixed, BS if inactive when $s_i$ is basic and SBS if inactive when $s_i$ is superbasic).

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** = Nag\_NoScale (default value is **options.scale** = Nag\_ExtraScale; see Section 12.2) is specified, the tests for assigning a key are applied to the variables of the scaled problem.

- A *Alternative optimum possible.*  $s_i$  is nonbasic, but its reduced gradient is essentially zero. This means that if  $s_i$  were allowed to start moving away from its bound, 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. However, if there are any degenerate variables (labelled D), the actual change might prove to be zero, since one of them could encounter a bound immediately. In either case, the values of the dual variables (or Lagrange multipliers) *might* also change.
- D *Degenerate.*  $s_i$  is basic or superbasic, but it is equal to (or very close to) one of its bounds.
- I *Infeasible.*  $s_i$  is basic or superbasic and is currently violating one of its bounds by more than the value of the optional argument **options.ftol** (default value =  $\max(10^{-6}, \sqrt{\epsilon})$ , where  $\epsilon$  is the *machine precision*; see Section 12.2).
- N *Not precisely optimal.*  $s_i$  is nonbasic or superbasic. If the value of the reduced gradient for  $s_i$  exceeds the value of the optional argument **options.optim\_tol** (default value =  $\max(10^{-6}, \sqrt{\epsilon})$ ; see Section 12.2), the solution would not be

declared optimal because the reduced gradient for  $s_i$  would not be considered negligible.

Activity	is the value of $v_i$ at the final iterate.
Slack Activity	is the value by which $v_i$ differs from its nearest bound. (For the free row (if any), it is set to Activity.)
Lower Bound	is the lower bound specified for $v_j$ . None indicates that $\mathbf{bl}[n+j-1] \leq -\mathbf{options.inf\_bound}$ , where <b>options.inf_bound</b> is the optional argument.
Upper Bound	is the upper bound specified for $v_j$ . None indicates that $\mathbf{bu}[n+j-1] \geq \mathbf{options.inf\_bound}$ .
Dual Activity	is the value of the dual variable $\pi_i$ (the Lagrange multiplier for $v_i$ ; see Section 11.3). For FP problems, $\pi_i$ is set to zero.
i	gives the index $i$ of $v_i$ .

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

If **options.print\_level** = Nag\_NoPrint then printout will be suppressed; you can print the final solution when nag\_opt\_sparse\_convex\_qp (e04nkc) returns to the calling program.

### 12.3.1 Output of results via a user-defined printing function

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

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

The rest of this section can be skipped if you wish to use the default printing facilities.

When a user-defined function is assigned to **options.print\_fun** this will be called in preference to the internal print function of nag\_opt\_sparse\_convex\_qp (e04nkc). Calls to the user-defined function are again controlled by means of the **options.print\_level** member. Information is provided through **st** and **comm**, the two structure arguments to **options.print\_fun**.

If **comm**→**it\_prt** = Nag\_TRUE then the results from the last iteration of nag\_opt\_sparse\_convex\_qp (e04nkc) are provided through **st**. Note that **options.print\_fun** will be called with **comm**→**it\_prt** = Nag\_TRUE only if **options.print\_level** = Nag\_Iter, Nag\_Iter\_Long, Nag\_Soln\_Iter, Nag\_Soln\_Iter\_Long or Nag\_Soln\_Iter\_Full.

The following members of **st** are set:

**iter** – Integer

The iteration count.

**qp** – Nag\_Boolean

Nag\_TRUE if a QP problem is being solved; Nag\_FALSE otherwise.

**pprice** – Integer

The partial price indicator.

**rgval** – double

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

**sb\_add** – Integer

The variable selected to enter the superbasic set.

**sb\_leave** – double

The variable chosen to leave the superbasic set.

**b\_leave** – Integer

The variable chosen to leave the basis (if any) to become nonbasic.

**bswap\_leave** – Integer

The variable chosen to leave the basis (if any) in a special basic  $\leftrightarrow$  superbasic swap.

**step** – double

The step length taken along the computed search direction.

**pivot** – double

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  $B$ .

**ninf** – Integer

The number of violated constraints or infeasibilities.

**f** – double

The current value of the objective function if **st** $\rightarrow$ **ninf** is zero; otherwise, the sum of the magnitudes of constraint violations.

**nnz\_l** – Integer

The number of nonzeros in the basis factor  $L$ .

**nnz\_u** – Integer

The number of nonzeros in the basis factor  $U$ .

**ncp** – Integer

The number of compressions of the basis factorization workspace carried out so far.

**norm\_rg** – double

The Euclidean norm of the reduced gradient at the start of the current iteration. This value is meaningful only if **st** $\rightarrow$ **qp** = Nag\_TRUE.

**nsb** – Integer

The number of superbasic variables. This value is meaningful only if **st** $\rightarrow$ **qp** = Nag\_TRUE.

**cond\_hz** – double

A lower bound on the condition number of the reduced Hessian. This value is meaningful only if **st** $\rightarrow$ **qp** = Nag\_TRUE.

If **comm** $\rightarrow$ **sol\_prt** = Nag\_TRUE then the final results for one row or column are provided through **st**. Note that **options.print\_fun** will be called with **comm** $\rightarrow$ **sol\_prt** = Nag\_TRUE only if **options.print\_level** = Nag\_Soln, Nag\_Soln.Iter, Nag\_Soln.Iter.Long or Nag\_Soln.Iter.Full. The following members of **st** are set (note that **options.print\_fun** is called repeatedly, for each row and column):

**m** – Integer

The number of rows (or general constraints) in the problem.

**n** – Integer

The number of columns (or variables) in the problem.

**col** – Nag\_Boolean

Nag\_TRUE if column information is being provided; Nag\_FALSE if row information is being provided.

**index** – Integer

If **st** $\rightarrow$ **col** = Nag\_TRUE then **st** $\rightarrow$ **index** is the index  $j$  (in the range  $1 \leq j \leq \mathbf{n}$ ) of the current column (variable) for which the remaining members of **st**, as described below, are set.

If  $\mathbf{st} \rightarrow \mathbf{col} = \text{Nag\_FALSE}$  then  $\mathbf{st} \rightarrow \mathbf{index}$  is the index  $i$  (in the range  $1 \leq i \leq \mathbf{m}$ ) of the current row (constraint) for which the remaining members of  $\mathbf{st}$ , as described below, are set.

**name** – char \*

The name of row  $i$  or column  $j$ .

**sstate** – char \*

$\mathbf{st} \rightarrow \mathbf{sstate}$  is a character string describing the state of row  $i$  or column  $j$ . This may be "LL", "UL", "EQ", "FR", "BS" or "SBS". The meaning of each of these is described in Section 12.3 (State).

**key** – char \*

$\mathbf{st} \rightarrow \mathbf{key}$  is a character string which gives additional information about the current row or column. The possible values of  $\mathbf{st} \rightarrow \mathbf{key}$  are: " ", "A", "D", "I" or "N". The meaning of each of these is described in Section 12.3 (State).

**val** – double

The activity of row  $i$  or column  $j$  at the final iterate.

**blo** – double

The lower bound on row  $i$  or column  $j$ .

**bup** – double

The upper bound on row  $i$  or column  $j$ .

**lmult** – double

The value of the Lagrange multiplier associated with the current row or column (i.e., the dual activity  $\pi_i$  for a row, or the reduced gradient  $d_j$  for a column) at the final iterate.

**objg** – double

The value of the objective gradient  $g_j$  at the final iterate.  $\mathbf{st} \rightarrow \mathbf{objg}$  is meaningful only when  $\mathbf{st} \rightarrow \mathbf{col} = \text{Nag\_TRUE}$  and should not be accessed otherwise. It is set to zero for FP problems.

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

**it\_prt** – Nag\_Boolean

Will be Nag\_TRUE when the print function is called with the result of the current iteration.

**sol\_prt** – Nag\_Boolean

Will be Nag\_TRUE when the print function is called with the final result.

**user** – double

**iuser** – Integer

**p** – Pointer

Pointers for communication of user information. If used they must be allocated memory either before entry to `nag_opt_sparse_convex_qp` (e04nkc) or during a call to `qphess` or **options.print\_fun**. The type Pointer will be `void *` with a C compiler that defines `void *` and `char *` otherwise.

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