

# NAG Toolbox for MATLAB

## e04ug

### 1 Purpose

e04ug solves sparse nonlinear programming problems.

### 2 Syntax

```
[a, ns, xs, istate, clamda, miniz, minz, ninf, sinf, obj, user, lwsav,
iwsav, rwsav, ifail] = e04ug(confun, objfun, n, m, ncnln, nonln, njnln,
iobj, a, ha, ka, bl, bu, start, names, ns, xs, istate, clamda, leniz,
lenz, lwsav, iwsav, rwsav, 'nnz', nnz, 'nname', nname, 'user', user)
```

Before calling e04ug, or the option setting function e04uj, e04wb **must** be called.

### 3 Description

e04ug is designed to solve a class of nonlinear programming problems that are assumed to be stated in the following general form:

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

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

The constraints involving  $F$  and  $Gx$  are called the *general constraints*. Note that upper and lower bounds are specified for all variables and constraints. This form allows full generality in specifying various types of constraint. In particular, the  $j$ th constraint can be defined as an *equality* by setting  $l_j = u_j$ . If certain bounds are not present, the associated elements of  $l$  or  $u$  can be set to special values that will be treated as  $-\infty$  or  $+\infty$ . (See the description of the optional parameter **Infinite Bound Size**.)

e04ug converts the upper and lower bounds on the  $m$  elements of  $F$  and  $Gx$  to equalities by introducing a set of *slack variables*  $s$ , where  $s = (s_1, s_2, \dots, s_m)^T$ . For example, the linear constraint  $5 \leq 2x_1 + 3x_2 \leq +\infty$  is replaced by  $2x_1 + 3x_2 - s_1 = 0$ , together with the bounded slack  $5 \leq s_1 \leq +\infty$ . The problem defined by (1) can therefore be re-written in the following equivalent form:

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

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

A basic variable ( $x_j$  say) is the  $j$ th variable associated with the  $j$ th column of the basis matrix  $B$ .

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

A superbasic variable is a nonbasic variable which is not at one of its bounds that is free to move in any desired direction (namely one that will improve the value of the objective function or reduce the sum of infeasibilities).

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

The optional parameter **Maximize** may be used to specify an alternative problem in which  $f(x)$  is maximized. If the objective function is nonlinear and all the constraints are linear,  $F$  is absent and the problem is said to be *linearly constrained*. In general, the objective and constraint functions are *structured* in the sense that they are formed from sums of linear and nonlinear functions. This structure can be exploited by the function during the solution process as follows.

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

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

subject to the constraints

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

and to the bounds

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

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

- the objective function is nonlinear. It is the sum of a *nonlinear* function of the variables ( $u, v, z$ ) and a *linear* function of the variables ( $z, w$ );
- the first two constraints are nonlinear. The third is linear;
- each nonlinear constraint function is the sum of a *nonlinear* function of the variables ( $u, v$ ) and a *linear* function of the variables ( $z, w$ ).

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

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

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

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

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

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

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

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

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

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

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

In general, the vectors  $x'$  and  $x''$  have different dimensions, but they *always overlap*, in the sense that the shorter vector is always the beginning of the other. In the above example, the nonlinear Jacobian variables  $(u, v)$  are an ordered subset of the nonlinear objective variables  $(u, v, z)$ . In other cases it could be the other way round (whichever is the most convenient), but the first way keeps  $J(x'')$  as small as possible.

Note that the nonlinear objective function  $f(x')$  may involve either a subset or superset of the variables appearing in the nonlinear constraint functions  $F(x'')$ . Thus, **nonln**  $\leq$  **njnl** (or vice-versa). Sometimes the objective and constraints really involve *disjoint sets of nonlinear variables*. In such cases the variables should be ordered so that **nonln**  $>$  **njnl** and  $x' = (x'', x''')$ , where the objective is nonlinear in just the last vector  $x'''$ . The first **njnl** elements of the gradient array **objgrd** should also be set to zero in (sub)program **objfun**. This is illustrated in Section 9.

If all elements of the constraint Jacobian are known (i.e., the optional parameter **Derivative Level** = 2 or 3), any constant elements may be assigned their correct values in **a**, **ha** and **ka**. The corresponding elements of the constraint Jacobian array **fjac** need not be reset in (sub)program **confun**. This includes values that are identically zero as constraint Jacobian elements are assumed to be zero unless specified otherwise. It must be emphasised that, if **Derivative Level** = 0 or 1, unassigned elements of **fjac** are *not* treated as constant; they are estimated by finite differences, at nontrivial expense.

If there are no nonlinear constraints in (1) and  $f(x)$  is linear or quadratic, then it may be more efficient to use e04nq to solve the resulting linear or quadratic programming problem, or one of e04mf, e04nc or e04nf if  $G$  is a *dense* matrix. If the problem is dense and does have nonlinear constraints then one of e04wd, e04uf or e04us (as appropriate) should be used instead.

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

e04ug is based on the SNOPT package described in Gill *et al.* 2002, which in turn utilizes functions from the MINOS package (see Murtagh and Saunders 1995). It incorporates a sequential quadratic programming (SQP) method that obtains search directions from a sequence of quadratic programming (QP) subproblems. Each QP subproblem minimizes a quadratic model of a certain Lagrangian function subject to a linearization of the constraints. An augmented Lagrangian merit function is reduced along each search direction to ensure convergence from any starting point. Further details can be found in Section 10.

Throughout this document the symbol  $\epsilon$  is used to represent the *machine precision* (see x02aj).

## 4 References

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Murtagh B A and Saunders M A 1995 MINOS 5.4 Users' Guide *Report SOL 83-20R* Department of Operations Research, Stanford University

Ortega J M and Rheinboldt W C 1970 *Iterative Solution of Nonlinear Equations in Several Variables* Academic Press

Powell M J D 1974 Introduction to constrained optimization *Numerical Methods for Constrained Optimization* (ed P E Gill and W Murray) 1–28 Academic Press

## 5 Parameters

### 5.1 Compulsory Input Parameters

1: **confun** – string containing name of m-file

**confun** must calculate the vector  $F(x)$  of nonlinear constraint functions and (optionally) its Jacobian  $\left( = \frac{\partial F}{\partial x} \right)$  for a specified  $n_1''$  ( $\leq n$ ) element vector  $x$ . If there are no nonlinear constraints (i.e., **ncnln** = 0), **confun** will never be called by e04ug and **confun** may be the string 'e04ugm'. **e04ugm** is included in the NAG Fortran Library. If there are nonlinear constraints, the first call to **confun** will occur before the first call to (sub)program **objfun**.

Its specification is:

```
[mode, f, fjac, user] = confun(mode, ncnln, njnln, nnzjac, x, fjac,
nstate, user)
```

#### Input Parameters

1: **mode** – int32 scalar

Indicates which values must be assigned during each call of **confun**. Only the following values need be assigned:

**mode** = 0

**f**.

**mode** = 1

All available elements of **fjac**.

**mode** = 2

**f** and all available elements of **fjac**.

You may set to a negative value as follows:

**mode**  $\leq -2$

The solution to the current problem is terminated and in this case e04ug will terminate with **ifail** set to **mode**.

**mode** = -1

The nonlinear constraint functions cannot be calculated at the current  $x$ . e04ug will then terminate with **ifail** = -1 unless this occurs during the linesearch; in this case, the linesearch will shorten the step and try again.

2: **ncnln** – int32 scalar

$n_N$ , the number of nonlinear constraints. These must be the first **ncnln** constraints in the problem.

3: **njnl** – int32 scalar

$n_1''$ , the number of nonlinear variables. These must be the first **njnl** variables in the problem.

4: **nnzjac** – int32 scalar

The number of nonzero elements in the constraint Jacobian. Note that **nnzjac** will usually be less than **ncnln** × **njnl**.

5: **x(njnl)** – double array

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

6: **fjac(nnzjac)** – double array

The elements of **fjac** are set to special values which enable e04ug to detect whether they are changed by **confun**.

If **mode** = 1 or 2, **fjac** must return the available elements of the constraint Jacobian evaluated at  $x$ . These elements must be stored in exactly the same positions as implied by the definitions of the arrays **a**, **ha** and **ka**. If optional parameter

**Derivative Level** = 2 or 3, the value of any constant Jacobian element not defined by **confun** will be obtained directly from **a**. Note that the function does not perform any internal checks for consistency (except indirectly via the optional parameter **Verify Level**), so great care is essential.

7: **nstate** – int32 scalar

If **nstate** = 1, then e04ug is calling **confun** for the first time. This parameter setting allows you to save computation time if certain data must be read or calculated only once.

If **nstate** ≥ 2, then e04ug is calling **confun** for the last time. This parameter setting allows you to perform some additional computation on the final solution. In general, the last call to **confun** is made with **nstate** = 2 + **ifail** (see Section 6).

Otherwise, **nstate** = 0.

8: **user** – Any MATLAB object

**confun** is called from e04ug with **user** as supplied to e04ug

### Output Parameters

1: **mode** – int32 scalar

Indicates which values must be assigned during each call of **confun**. Only the following values need be assigned:

**mode** = 0

**f**.

**mode** = 1

All available elements of **fjac**.

**mode** = 2

**f** and all available elements of **fjac**.

You may set to a negative value as follows:

**mode** ≤ −2

The solution to the current problem is terminated and in this case e04ug will terminate with **ifail** set to **mode**.

**mode** = −1

The nonlinear constraint functions cannot be calculated at the current  $x$ . e04ug will then terminate with **ifail** = −1 unless this occurs during the linesearch; in this case, the linesearch will shorten the step and try again.

2: **f(ncnln)** – double array

If **mode** = 0 or 2, **f**( $i$ ) must contain the value of the  $i$ th nonlinear constraint function at  $x$ .

3: **fjac(nnzjac)** – double array

The elements of **fjac** are set to special values which enable e04ug to detect whether they are changed by **confun**.

If **mode** = 1 or 2, **fjac** must return the available elements of the constraint Jacobian evaluated at  $x$ . These elements must be stored in exactly the same positions as implied by the definitions of the arrays **a**, **ha** and **ka**. If optional parameter

**Derivative Level** = 2 or 3, the value of any constant Jacobian element not defined by **confun** will be obtained directly from **a**. Note that the function does not perform any internal checks for consistency (except indirectly via the optional parameter **Verify Level**), so great care is essential.

4: **user** – Any MATLAB object

**confun** is called from e04ug with **user** as supplied to e04ug

2: **objfun** – string containing name of m-file

**objfun** must calculate the nonlinear part of the objective function  $f(x)$  and (optionally) its gradient  $\left(\frac{\partial f}{\partial x}\right)$  for a specified  $n'_1$  ( $\leq n$ ) element vector  $x$ . If there are no nonlinear objective variables (i.e., **nonln** = 0), **objfun** will never be called by e04ug and **objfun** may be the string 'e04ugn'. **e04ugn** is included in the NAG Fortran Library.

Its specification is:

```
[mode, objf, objgrd, user] = objfun(mode, nonln, x, objgrd, nstate, user)
```

**Input Parameters**

1: **mode** – int32 scalar

Indicates which values must be assigned during each call of **objfun**. Only the following values need be assigned:

**mode** = 0

**objf**.

**mode** = 1

All available elements of **objgrd**.

**mode** = 2

**objf** and all available elements of **objgrd**.

You may set to a negative value as follows:

**mode**  $\leq$  -2

The solution to the current problem is terminated and in this case e04ug will terminate with **ifail** set to **mode**.

**mode** = -1

The nonlinear part of the objective function cannot be calculated at the current  $x$ . e04ug will then terminate with **ifail** = -1 unless this occurs during the linesearch; in this case, the linesearch will shorten the step and try again.

2: **nonln** – int32 scalar

$n'_1$ , the number of nonlinear objective variables. These must be the first **nonln** variables in the problem.

3: **x(nonln)** – double array

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

4: **objgrd(nonln)** – double array

The elements of **objgrd** are set to special values which enable e04ug to detect whether they are changed by **objfun**.

If **mode** = 1 or 2, **objgrd** must return the available elements of the gradient evaluated at  $x$ .

5: **nstate** – int32 scalar

If **nstate** = 1, e04ug is calling **objfun** for the first time. This parameter setting allows you to save computation time if certain data must be read or calculated only once.

If **nstate**  $\geq$  2, e04ug is calling **objfun** for the last time. This parameter setting allows you to perform some additional computation on the final solution. In general, the last call to **objfun** is made with **nstate** = 2 + **ifail** (see Section 6).

Otherwise, **nstate** = 0.

6: **user** – Any MATLAB object

**objfun** is called from e04ug with **user** as supplied to e04ug

### Output Parameters

1: **mode** – int32 scalar

Indicates which values must be assigned during each call of **objfun**. Only the following values need be assigned:

**mode** = 0

**objf**.

**mode** = 1

All available elements of **objgrd**.

**mode** = 2

**objf** and all available elements of **objgrd**.

You may set to a negative value as follows:

**mode**  $\leq -2$

The solution to the current problem is terminated and in this case e04ug will terminate with **ifail** set to **mode**.

**mode** = -1

The nonlinear part of the objective function cannot be calculated at the current  $x$ . e04ug will then terminate with **ifail** = -1 unless this occurs during the linesearch; in this case, the linesearch will shorten the step and try again.

2: **objf** – double scalar

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

3: **objgrd(nonln)** – double array

The elements of **objgrd** are set to special values which enable e04ug to detect whether they are changed by **objfun**.

If **mode** = 1 or 2, **objgrd** must return the available elements of the gradient evaluated at  $x$ .

4: **user** – Any MATLAB object

**objfun** is called from e04ug with **user** as supplied to e04ug

3: **n** – int32 scalar

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

*Constraint:*  $n \geq 1$ .

4: **m** – int32 scalar

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

*Constraint:*  $m \geq 1$ .

5: **ncnln** – int32 scalar

$n_N$ , the number of nonlinear constraints.

*Constraint:*  $0 \leq \text{ncnln} \leq m$ .

6: **nonln** – int32 scalar

$n'_1$ , the number of nonlinear objective variables. If the objective function is nonlinear, the leading  $n'_1$  columns of  $A$  belong to the nonlinear objective variables. (See also the description for **njnln**.)

*Constraint:*  $0 \leq \text{nonln} \leq n$ .

7: **njnln** – int32 scalar

$n''_1$ , the number of nonlinear Jacobian variables. If there are any nonlinear constraints, the leading  $n''_1$  columns of  $A$  belong to the nonlinear Jacobian variables. If  $n'_1 > 0$  and  $n''_1 > 0$ , the nonlinear



objective and Jacobian variables overlap. The total number of nonlinear variables is given by  $\bar{n} = \max(n'_1, n''_1)$ .

*Constraints:*

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

8: **iobj – int32 scalar**

If **iobj** > **ncnln**, row **iobj** of  $A$  is a free row containing the nonzero elements of the linear part of the objective function.

**iobj** = 0

There is no free row.

**iobj** = -1

There is a dummy ‘free’ row.

*Constraints:*

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

9: **a(nnz) – double array**

The nonzero elements of the Jacobian matrix  $A$ , ordered by increasing column index. Since the constraint Jacobian matrix  $J(x'')$  must always appear in the top left-hand corner of  $A$ , those elements in a column associated with any nonlinear constraints must come before any elements belonging to the linear constraint matrix  $G$  and the free row (if any; see **iobj**).

In general, **a** is partitioned into a nonlinear part and a linear part corresponding to the nonlinear variables and linear variables in the problem. Elements in the nonlinear part may be set to any value (e.g., zero) because they are initialized at the first point that satisfies the linear constraints and the upper and lower bounds.

If **Derivative Level** = 2 or 3, the nonlinear part may also be used to store any constant Jacobian elements. Note that if (sub)program **confun** does not define the constant Jacobian element **fjac**( $i$ ) then the missing value will be obtained directly from **a**( $j$ ) for some  $j \geq i$ .

If **Derivative Level** = 0 or 1, unassigned elements of **fjac** are *not* treated as constant; they are estimated by finite differences, at nontrivial expense.

The linear part must contain the nonzero elements of  $G$  and the free row (if any). If **iobj** = -1, set **a**(1) = 0. Elements with the same row and column indices are not allowed. (See also the descriptions for **ha** and **ka**.)

10: **ha(nnz) – int32 array**

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

*Constraint:*  $1 \leq \mathbf{ha}(i) \leq \mathbf{m}$ , for  $i = 1, 2, \dots, \mathbf{nnz}$ .

11: **ka(n + 1) – int32 array**

**ka**( $j$ ) must contain the index in **a** of the start of the  $j$ th column, for  $j = 1, 2, \dots, \mathbf{n}$ . To specify the  $j$ th column as empty, set **ka**( $j$ ) = **ka**( $j + 1$ ). Note that the first and last elements of **ka** must be such that **ka**(1) = 1 and **ka**( $\mathbf{n} + 1$ ) = **nnz** + 1. If **iobj** = -1, set **ka**( $j$ ) = 2, for  $j = 2, 3, \dots, \mathbf{n}$ .

*Constraints:*

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

12: **bl(n + m) – double array**

$l$ , the lower bounds for all the variables and general constraints, in the following order. The first  $\mathbf{n}$  elements of **bl** must contain the bounds on the variables  $x$ , the next **ncnln** elements the bounds for the nonlinear constraints  $F(x)$  (if any) and the next  $(\mathbf{m} - \mathbf{ncnln})$  elements the bounds for the linear constraints  $Gx$  and the free row (if any). To specify a nonexistent lower bound (i.e.,  $l_j = -\infty$ ), set **bl**( $j$ )  $\leq -\mathit{bigbnd}$ . To specify the  $j$ th constraint as an *equality*, set **bl**( $j$ ) = **bu**( $j$ ) =  $\beta$ , say, where  $|\beta| < \mathit{bigbnd}$ . If **iobj** = -1, set **bl**( $\mathbf{n} + \mathbf{abs}(\mathbf{iobj})$ )  $\leq -\mathit{bigbnd}$ .

*Constraint:* if **ncnln** < **iobj**  $\leq \mathbf{m}$  or **iobj** = -1, **bl**( $\mathbf{n} + \mathbf{abs}(\mathbf{iobj})$ )  $\leq -\mathit{bigbnd}$ .

(See also the description for **bu**.)

13: **bu(n + m) – double array**

$u$ , the upper bounds for all the variables and general constraints, in the following order. The first  $\mathbf{n}$  elements of **bu** must contain the bounds on the variables  $x$ , the next **ncnln** elements the bounds for the nonlinear constraints  $F(x)$  (if any) and the next  $(\mathbf{m} - \mathbf{ncnln})$  elements the bounds for the linear constraints  $Gx$  and the free row (if any). To specify a nonexistent upper bound (i.e.,  $u_j = +\infty$ ), set **bu**( $j$ )  $\geq \mathit{bigbnd}$ . To specify the  $j$ th constraint as an *equality*, set **bu**( $j$ ) = **bl**( $j$ ) =  $\beta$ , say, where  $|\beta| < \mathit{bigbnd}$ . If **iobj** = -1, set **bu**( $\mathbf{n} + \mathbf{abs}(\mathbf{iobj})$ )  $\geq \mathit{bigbnd}$ .

*Constraints:*

$$\begin{aligned} &\text{if } \mathbf{ncnln} < \mathbf{iobj} \leq \mathbf{m} \text{ or } \mathbf{iobj} = -1, \mathbf{bu}(\mathbf{n} + \mathbf{abs}(\mathbf{iobj})) \geq \mathit{bigbnd}; \\ &\mathbf{bl}(j) \leq \mathbf{bu}(j), \text{ for } j = 1, 2, \dots, \mathbf{n} + \mathbf{m}; \\ &\text{if } \mathbf{bl}(j) = \mathbf{bu}(j) = \beta, |\beta| < \mathit{bigbnd}. \end{aligned}$$

14: **start – string**

Indicates how a starting basis is to be obtained.

**start** = 'C'

An internal Crash procedure will be used to choose an initial basis.

**start** = 'W'

A basis is already defined in **istate** and **ns** (probably from a previous call).

*Constraint:* **start** = 'C' or 'W'.

15: **names(nname) – string array**

Specifies the column and row names to be used in the printed output.

If **nname** = 1, **names** is not referenced and the printed output will use default names for the columns and rows.

If **nname** =  $\mathbf{n} + \mathbf{m}$ , the first  $\mathbf{n}$  elements must contain the names for the columns, the next **ncnln** elements must contain the names for the nonlinear rows (if any) and the next  $(\mathbf{m} - \mathbf{ncnln})$  elements must contain the names for the linear rows (if any) to be used in the printed output. Note that the name for the free row or dummy 'free' row must be stored in **names**( $\mathbf{n} + \mathbf{abs}(\mathbf{iobj})$ ).

16: **ns – int32 scalar**

$n_S$ , the number of superbasics. It need not be specified if **start** = 'C', but must retain its value from a previous call when **start** = 'W'.

17: **xs(n + m) – double array**

The initial values of the variables and slacks  $(x, s)$ . (See the description for **istate**.)

18: **istate(n + m) – int32 array**

If **start** = 'C', the first **n** elements of **istate** and **xs** must specify the initial states and values, respectively, of the variables  $x$ . (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  $(A \ -I)$ . Possible values for **istate**( $j$ ) are as follows:

**istate**( $j$ )    **State of xs**( $j$ ) **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 **istate**( $j$ ) = 0 and **xs**( $j$ ) = 0.0, for  $j = 1, 2, \dots, n$ . All variables will then be eligible for the initial basis. Less trivially, to say that the  $j$ th variable will probably be equal to one of its bounds, set **istate**( $j$ ) = 4 and **xs**( $j$ ) = **bl**( $j$ ) or **istate**( $j$ ) = 5 and **xs**( $j$ ) = **bu**( $j$ ) as appropriate.

Following the Crash procedure, variables for which **istate**( $j$ ) = 2 are made superbasic. Other variables not selected for the basis are then made nonbasic at the value **xs**( $j$ ) if **bl**( $j$ ) ≤ **xs**( $j$ ) ≤ **bu**( $j$ ), or at the value **bl**( $j$ ) or **bu**( $j$ ) closest to **xs**( $j$ ).

If **start** = 'W', **istate** and **xs** must specify the initial states and values, respectively, of the variables and slacks  $(x, s)$ . If the function has been called previously with the same values of **n** and **m**, **istate** already contains satisfactory information.

*Constraints:*

if **start** = 'C',  $0 \leq \text{istate}(j) \leq 5$ , for  $j = 1, 2, \dots, n$ ;  
if **start** = 'W',  $0 \leq \text{istate}(j) \leq 3$ , for  $j = 1, 2, \dots, n + m$ .

19: **clamda(n + m) – double array**

If **ncnln** > 0, **clamda**( $j$ ) must contain a Lagrange multiplier estimate for the  $j$ th nonlinear constraint  $F_j(x)$ , for  $j = n + 1, n + 2, \dots, n + \text{ncnln}$ . If nothing special is known about the problem, or there is no wish to provide special information, you may set **clamda**( $j$ ) = 0.0. The remaining elements need not be set.

20: **leniz – int32 scalar**

*Constraint:* **leniz** ≥ max(500, **n + m**).

21: **lenz – int32 scalar**

*Constraint:* **lenz** ≥ 500.

The amounts of workspace provided (i.e., **leniz** and **lenz**) and required (i.e., **miniz** and **minz**) are (by default) output on the current advisory message unit (as defined by x04ab). Since the minimum values of **leniz** and **lenz** required to start solving the problem are returned in **miniz** and **minz** respectively, you may prefer to obtain appropriate values from the output of a preliminary run with **leniz** set to max(500, **n + m**) and/or **lenz** set to 500. (e04ug will then terminate with **ifail** = 15 or 16.)

22: **lwsav(20) – logical array**23: **iwsav(550) – int32 array**24: **rwsav(550) – double array**

The arrays **lwsav**, **iwsav** and **rwsav** **must not** be altered between calls to any of the functions e04wb, e04ug, e04uj.

## 5.2 Optional Input Parameters

### 1: **nnz** – int32 scalar

*Default:* The dimension of the arrays **a**, **ha**. (An error is raised if these dimensions are not equal.)  
the number of nonzero elements in  $A$  (including the Jacobian for any nonlinear constraints). If **iobj** = -1, set **nnz** = 1.

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

### 2: **nname** – int32 scalar

*Default:* The dimension of the array **names**.

the number of column (i.e., variable) and row (i.e., constraint) names supplied in **names**.

**nname** = 1

There are no names. Default names will be used in the printed output.

**nname** = **n** + **m**

All names must be supplied.

*Constraint:* **nname** = 1 or **n** + **m**.

### 3: **user** – Any MATLAB object

**user** is not used by e04ug, but is passed to **confun** and **objfun**. Note that for large objects it may be more efficient to use a global variable which is accessible from the m-files than to use **user**.

## 5.3 Input Parameters Omitted from the MATLAB Interface

iz, z

## 5.4 Output Parameters

### 1: **a(nnz)** – double array

Elements in the nonlinear part corresponding to nonlinear Jacobian variables are overwritten.

### 2: **ns** – int32 scalar

The final number of superbasics.

### 3: **xs(n + m)** – double array

The final values of the variables and slacks  $(x, s)$ .

### 4: **istate(n + m)** – int32 array

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

<b>istate</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 **ninf** = 0, basic and superbasic variables may be outside their bounds by as much as the value of the optional parameter **Minor Feasibility Tolerance**. Note that if scaling is specified, the optional parameter **Minor Feasibility Tolerance** 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 the optional parameter **Minor Feasibility Tolerance** and there may be some nonbasic variables for which **xs(j)** lies strictly between its bounds.

If **ninf** > 0, some basic and superbasic variables may be outside their bounds by an arbitrary amount (bounded by **sinf** if scaling was not used).

5: **clamda(n + m) – double array**

A set of Lagrange multipliers for the bounds on the variables (*reduced costs*) and the general constraints (*shadow costs*). More precisely, the first **n** elements contain the multipliers for the bounds on the variables, the next **ncnln** elements contain the multipliers for the nonlinear constraints  $F(x)$  (if any) and the next **(m – ncnln)** elements contain the multipliers for the linear constraints  $Gx$  and the free row (if any).

6: **miniz – int32 scalar**

The minimum value of **leniz** required to start solving the problem. If **ifail** = 12, e04ug may be called again with **leniz** suitably larger than **miniz**. (The bigger the better, since it is not certain how much workspace the basis factors need.)

7: **minz – int32 scalar**

The minimum value of **lenz** required to start solving the problem. If **ifail** = 13, e04ug may be called again with **lenz** suitably larger than **minz**. (The bigger the better, since it is not certain how much workspace the basis factors need.)

8: **ninf – int32 scalar**

The number of constraints that lie outside their bounds by more than the value of the optional parameter **Minor Feasibility Tolerance**.

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

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

9: **sinf – double scalar**

The sum of the infeasibilities of constraints that lie outside their bounds by more than the value of the optional parameter **Minor Feasibility Tolerance**.

10: **obj – double scalar**

The value of the objective function.

11: **user – Any MATLAB object**

**user** is not used by e04ug, but is passed to **confun** and **objfun**. Note that for large objects it may be more efficient to use a global variable which is accessible from the m-files than to use **user**.

12: **lwsav(20) – logical array**

13: **iwsav(550) – int32 array**

14: **rwsav(550) – double array**

The arrays **lwsav**, **iwsav** and **rwsav** **must not** be altered between calls to any of the functions e04wb, e04ug, e04uj.

15: **ifail** – int32 scalar

0 unless the function detects an error (see Section 6).

## 6 Error Indicators and Warnings

**Note:** e04ug may return useful information for one or more of the following detected errors or warnings.

**ifail** < 0

A negative value of **ifail** indicates an exit from e04ug because you set **mode** < 0 in the user-supplied (sub)programs **objfun** or **confun**. The value of **ifail** will be the same as your setting of **mode**.

**ifail** = 1

The problem is infeasible. The general constraints cannot all be satisfied simultaneously to within the values of the optional parameters **Major Feasibility Tolerance** (default value =  $\sqrt{\epsilon}$ ) and **Minor Feasibility Tolerance** (default value =  $\sqrt{\epsilon}$ ).

**ifail** = 2

The problem is unbounded (or badly scaled). The objective function is not bounded below (or above in the case of maximization) in the feasible region because a nonbasic variable can apparently be increased or decreased by an arbitrary amount without causing a basic variable to violate a bound. Add an upper or lower bound to the variable (whose index is printed by default by e04ug) and rerun e04ug.

**ifail** = 3

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

**ifail** = 4

Too many iterations. The values of the optional parameters **Major Iteration Limit** (default value = 1000) and/or **Iteration Limit** (default value = 10000) are too small.

**ifail** = 5

Feasible solution found, but requested accuracy could not be achieved. Check that the value of the optional parameter **Major Optimality Tolerance** (default value =  $\sqrt{\epsilon}$ ) is not too small (say,  $< \epsilon$ ).

**ifail** = 6

The value of the optional parameter **Superbasics Limit** (default value =  $\min(500, \bar{n} + 1)$ ) is too small.

**ifail** = 7

An input parameter is invalid.

**ifail** = 8

The user-supplied derivatives of the objective function computed by (sub)program **objfun** appear to be incorrect. Check that **objfun** has been coded correctly and that all relevant elements of the objective gradient have been assigned their correct values.

**ifail = 9**

The user-supplied derivatives of the nonlinear constraint functions computed by (sub)program **confun** appear to be incorrect. Check that **confun** has been coded correctly and that all relevant elements of the nonlinear constraint Jacobian have been assigned their correct values.

**ifail = 10**

The current point cannot be improved upon. Check that (sub)program **objfun** and (sub)program **confun** have been coded correctly and that they are consistent with the value of the optional parameter **Derivative Level** (default value = 3).

**ifail = 11**

Numerical error in trying to satisfy the linear constraints (or the linearized nonlinear constraints). The basis is very ill-conditioned.

**ifail = 12**

Not enough integer workspace for the basis factors. Increase **leniz** and rerun e04ug.

**ifail = 13**

Not enough real workspace for the basis factors. Increase **lenz** and rerun e04ug.

**ifail = 14**

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

**ifail = 15**

Not enough integer workspace to start solving the problem. Increase **leniz** to at least **miniz** and rerun e04ug.

**ifail = 16**

Not enough real workspace to start solving the problem. Increase **lenz** to at least **minz** and rerun e04ug.

**ifail = 17**

An unexpected error has occurred. Please contact NAG.

## 7 Accuracy

If the value of the optional parameter **Major Optimality Tolerance** is set to  $10^{-d}$  (default value =  $\sqrt{\epsilon}$ ) and **ifail** = 0 on exit, then the final value of  $f(x)$  should have approximately  $d$  correct significant digits.

## 8 Further Comments

This section contains a description of the printed output.

### 8.1 Major Iteration Printout

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

**Maj** is the major iteration count.

**Mnr** is the number of minor iterations required by the feasibility and optimality phases of the QP subproblem. Generally, **Mnr** will be 1 in the later iterations, since theoretical

analysis predicts that the correct active set will be identified near the solution (see Section 10).

Note that `Mnr` may be greater than the optional parameter **Minor Iteration Limit** if some iterations are required for the feasibility phase.

Step	is the step $\alpha_k$ taken along the computed search direction. On reasonably well-behaved problems, the unit step (i.e., $\alpha_k = 1$ ) will be taken as the solution is approached.
Merit Function	<p>is the value of the augmented Lagrangian merit function (6) at the current iterate. This function will decrease at each iteration unless it was necessary to increase the penalty parameters (see Section 8.1). As the solution is approached, Merit Function will converge to the value of the objective function at the solution.</p> <p>In elastic mode (see Section 10.2) then the merit function is a composite function involving the constraint violations weighted by the value of the optional parameter <b>Elastic Weight</b>.</p> <p>If there are no nonlinear constraints present then this entry contains <b>Objective</b>, the value of the objective function <math>f(x)</math>. In this case, <math>f(x)</math> will decrease monotonically to its optimal value.</p>
Feasibl	<p>is the value of <code>rowerr</code>, the largest element of the scaled nonlinear constraint residual vector defined in the description of the optional parameter <b>Major Feasibility Tolerance</b>. The solution is regarded as ‘feasible’ if <code>Feasibl</code> is less than (or equal to) the optional parameter <b>Major Feasibility Tolerance</b>. <code>Feasibl</code> will be approximately zero in the neighbourhood of a solution.</p> <p>If there are no nonlinear constraints present, all iterates are feasible and this entry is not printed.</p>
Optimal	is the value of <code>maxgap</code> , the largest element of the maximum complementarity gap vector defined in the description of the optional parameter <b>Major Optimality Tolerance</b> . The Lagrange multipliers are regarded as ‘optimal’ if <code>Optimal</code> is less than (or equal to) the optional parameter <b>Major Optimality Tolerance</b> . <code>Optimal</code> will be approximately zero in the neighbourhood of a solution.
Cond Hz	is an estimate of the condition number of the reduced Hessian of the Lagrangian (not printed if <code>ncnln</code> and <code>nonln</code> are both zero). It is the square of the ratio between the largest and smallest diagonal elements of the upper triangular matrix $R$ . This constitutes a lower bound on the condition number of the matrix $R^T R$ that approximates the reduced Hessian. The larger this number, the more difficult the problem.
PD	is a two-letter indication of the status of the convergence tests involving the feasibility and optimality of the iterates defined in the descriptions of the optional parameters <b>Major Feasibility Tolerance</b> and <b>Major Optimality Tolerance</b> . Each letter is T if the test is satisfied and F otherwise. The tests indicate whether the values of <code>Feasibl</code> and <code>Optimal</code> are sufficiently small. For example, TF or TT is printed if there are no nonlinear constraints present (since all iterates are feasible). If either indicator is F when e04ug terminates with <code>ifail = 0</code> , you should check the solution carefully.
M	is printed if an extra evaluation of user-supplied (sub)programs <b>objfun</b> and <b>confun</b> was needed in order to define an acceptable positive-definite quasi-Newton update to the Hessian of the Lagrangian. This modification is only performed when there are nonlinear constraints present.
m	is printed if, in addition, it was also necessary to modify the update to include an augmented Lagrangian term.
s	is printed if a self-scaled BFGS (Broyden–Fletcher–Goldfarb–Shanno) update was performed. This update is always used when the Hessian approximation is diagonal and hence always follows a Hessian reset.



S	is printed if, in addition, it was also necessary to modify the self-scaled update in order to maintain positive-definiteness.
n	is printed if no positive-definite BFGS update could be found, in which case the approximate Hessian is unchanged from the previous iteration.
r	is printed if the approximate Hessian was reset after 10 consecutive major iterations in which no BFGS update could be made. The diagonal elements of the approximate Hessian are retained if at least one update has been performed since the last reset. Otherwise, the approximate Hessian is reset to the identity matrix.
R	is printed if the approximate Hessian has been reset by discarding all but its diagonal elements. This reset will be forced periodically by the values of the optional parameters <b>Hessian Frequency</b> and <b>Hessian Updates</b> . However, it may also be necessary to reset an ill-conditioned Hessian from time to time.
l	is printed if the change in the norm of the variables was greater than the value defined by the optional parameter <b>Major Step Limit</b> . If this output occurs frequently during later iterations, it may be worthwhile increasing the value of <b>Major Step Limit</b> .
c	is printed if central differences have been used to compute the unknown elements of the objective and constraint gradients. A switch to central differences is made if either the linesearch gives a small step, or $x$ is close to being optimal. In some cases, it may be necessary to re-solve the QP subproblem with the central difference gradient and Jacobian.
u	is printed if the QP subproblem was unbounded.
t	is printed if the minor iterations were terminated after the number of iterations specified by the value of the optional parameter <b>Minor Iteration Limit</b> was reached.
i	is printed if the QP subproblem was infeasible when the function was not in elastic mode. This event triggers the start of nonlinear elastic mode, which remains in effect for all subsequent iterations. Once in elastic mode, the QP subproblems are associated with the elastic problem (8) (see Section 10.2). It is also printed if the minimizer of the elastic subproblem does not satisfy the linearized constraints when the function is already in elastic mode. (In this case, a feasible point for the usual QP subproblem may or may not exist.)
w	is printed if a weak solution of the QP subproblem was found.

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

The following describes the printout for each variable. A full stop (.) is printed for any numerical value that is zero.

Variable	gives the name of the variable. If <b>nname</b> = 1, a default name is assigned to the $j$ th variable for $j = 1, 2, \dots, n$ . If <b>nname</b> = <b>n</b> + <b>m</b> , the name supplied in <b>names(j)</b> is assigned to the $j$ th variable.
State	gives the state of the variable (LL if nonbasic on its lower bound, UL if nonbasic on its upper bound, EQ if nonbasic and fixed, FR if nonbasic and strictly between its bounds, BS if basic and SBS if superbasic).  A key is sometimes printed before State. Note that unless the optional parameter <b>Scale Option</b> = 0 is specified, the tests for assigning a key are applied to the variables of the scaled problem.  A <i>Alternative optimum possible</i> . The variable is nonbasic, but its reduced gradient is essentially zero. This means that if the variable were allowed to start moving away from its current value, there would be no change in the value of the objective function. The values of the basic and superbasic

variables *might* change, giving a genuine alternative solution. The values of the Lagrange multipliers *might* also change.

- D *Degenerate.* The variable is basic, but it is equal to (or very close to) one of its bounds.
- I *Infeasible.* The variable is basic and is currently violating one of its bounds by more than the value of the optional parameter **Minor Feasibility Tolerance**.
- N *Not precisely optimal.* The variable is nonbasic. Its reduced gradient is larger than the value of the optional parameter **Major Feasibility Tolerance**.

Value	is the value of the variable at the final iteration.
Lower Bound	is the lower bound specified for the variable. None indicates that $\mathbf{bl}(j) \leq -bigbnd$ .
Upper Bound	is the upper bound specified for the variable. None indicates that $\mathbf{bu}(j) \geq bigbnd$ .
Lagr Mult	is the Lagrange multiplier for the associated bound. This will be zero if State is FR. If $x$ is optimal, the multiplier should be nonnegative if State is LL, nonpositive 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 $\mathbf{bl}(j)$ and $\mathbf{bu}(j)$ . A blank entry indicates that the associated variable is not bounded (i.e., $\mathbf{bl}(j) \leq -bigbnd$ and $\mathbf{bu}(j) \geq bigbnd$ ).

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  $m$ ,  $\mathbf{names}(j)$  replaced by  $\mathbf{names}(n+j)$ ,  $\mathbf{bl}(j)$  and  $\mathbf{bu}(j)$  are replaced by  $\mathbf{bl}(n+j)$  and  $\mathbf{bu}(n+j)$  respectively. The heading is changed as follows:

Constrnt            gives the name of the general constraint.

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

## 8.2 Minor Iteration Printout

This section describes the printout produced by the minor iterations of e04ug, which involve solving a QP subproblem at every major iteration. (Further details can be found in Section 8.1.) The printout is a subset of the monitoring information produced by the function at every iteration (see Section 12). You can control the level of printed output (see the description of the optional parameter **Minor Print Level**). Note that the printout is produced only if **Minor Print Level**  $\geq 1$  (default value = 0, which produces no output).

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

Itn	is the iteration count.
Step	is the step taken along the computed search direction.
Ninf	is the number of infeasibilities. This will not increase unless the iterations are in elastic mode. Ninf will be zero during the optimality phase.
Sinf	is the value of the sum of infeasibilities if Ninf is nonzero. This will be zero during the optimality phase.
Objective	is the value of the current QP objective function when Ninf is zero and the iterations are not in elastic mode. The switch to elastic mode is indicated by a change in the heading to Composite Obj.
Composite Obj	is the value of the composite objective function (9) when the iterations are in elastic mode. This function will decrease monotonically at each iteration.
Norm rg	is the Euclidean norm of the reduced gradient of the QP objective function. During the optimality phase, this norm will be approximately zero after a unit step.

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

## 9 Example

e04ug\_confun.m

```
function [mode, f, fjac, user] = ...
    confun(mode, ncnln, njnln, nnzjac, x, fjac, nstate, user)
    f = zeros(ncnln, 1);

    if (mode == 0 || mode == 2)
        f(1) = 1000*sin(-x(1)-0.25) + 1000*sin(-x(2)-0.25);
        f(2) = 1000*sin(x(1)-0.25) + 1000*sin(x(1)-x(2)-0.25);
        f(3) = 1000*sin(x(2)-x(1)-0.25) + 1000*sin(x(2)-0.25);
    end

    if (mode == 1 || mode == 2)
        % nonlinear jacobian elements for column 1.
        fjac(1) = -1000*cos(-x(1)-0.25);
        fjac(2) = 1000*cos(x(1)-0.25) + 1000*cos(x(1)-x(2)-0.25);
        fjac(3) = -1000*cos(x(2)-x(1)-0.25);
        % nonlinear jacobian elements for column 2.
        fjac(4) = -1000*cos(-x(2)-0.25);
        fjac(5) = -1000*cos(x(1)-x(2)-0.25);
        fjac(6) = 1000*cos(x(2)-x(1)-0.25) + 1000*cos(x(2) -0.25);
    end
```

e04ug\_objfun.m

```
function [mode, objf, objgrd, user] = objfun(mode, nonln, x, objgrd,
    nstate, user)

    if (mode == 0 || mode == 2)
        objf = 1.0e-6*x(3)^3 + 2.0e-6*x(4)^3/3;
    end

    if (mode == 1 || mode == 2)
        objgrd(1) = 0;
        objgrd(2) = 0;
        objgrd(3) = 3.0e-6*x(3)^2;
        objgrd(4) = 2.0e-6*x(4)^2;
    end
```

```
n = int32(4);
m = int32(6);
ncnln = int32(3);
nonln = int32(4);
njnln = int32(2);
iobj = int32(6);
a = [9.999999999999999e+24;
     9.999999999999999e+24;
     9.999999999999999e+24;
     1;
     -1;
     9.999999999999999e+24;
     9.999999999999999e+24;
     9.999999999999999e+24;
     -1;
     1;
     3;
     -1;
     -1;
     2];
```

```

ha = [int32(1);
      int32(2);
      int32(3);
      int32(5);
      int32(4);
      int32(1);
      int32(2);
      int32(3);
      int32(5);
      int32(4);
      int32(6);
      int32(1);
      int32(2);
      int32(6)];
ka = [int32(1);
      int32(6);
      int32(11);
      int32(13);
      int32(15)];
bl = [-0.55;
      -0.55;
      0;
      0;
      -894.8;
      -894.8;
      -1294.8;
      -0.55;
      -0.55;
      -9.999999999999999e+24];
bu = [0.55;
      0.55;
      1200;
      1200;
      -894.8;
      -894.8;
      -1294.8;
      9.999999999999999e+24;
      9.999999999999999e+24;
      9.999999999999999e+24];
start = 'C';
names = {'Varble 1'; 'Varble 2'; 'Varble 3'; 'Varble 4'; 'NlnCon 1';
         'NlnCon 2'; 'NlnCon 3'; 'LinCon 1'; 'LinCon 2'; 'Free Row'};
ns = int32(0);
xs = [0;
      0;
      0;
      0;
      0;
      0;
      0;
      0;
      0;
      0;
      0];
istate = zeros(10, 1, 'int32');
clamda = [0;
          0;
          0;
          0;
          0;
          0;
          0;
          0;
          0;
          0];
leniz = int32(1000);
lenz = int32(1000);
[cwsav,lwsav,iwsav,rwsav,ifail] = e04wb('e04ug');
[aOut, nsOut, xsOut, istateOut, clamdaOut, miniz, minz, ninf, sinf, obj,
...
 user, lwsavOut, iwsavOut, rwsavOut, ifail] = ...

```

```

e04ug('e04ug_confun', 'e04ug_objfun', n, m, ncnln, nonln, njnln, ...
      iobj, a, ha, ka, bl, bu, start, names, ns, xs, istate, ...
      clamda, leniz, lenz, lwsav, iwsav, rwsav)

aOut =
    1.0e+03 *
    -0.9327
     1.9565
    -0.7213
     0.0010
    -0.0010
    -0.9893
    -0.9651
     1.5197
    -0.0010
     0.0010
     0.0030
    -0.0010
    -0.0010
     0.0020
nsOut =
         1
xsOut =
    1.0e+03 *
     0.0001
    -0.0004
     0.6799
     1.0261
    -0.8948
    -0.8948
    -1.2948
    -0.0005
     0.0005
     4.0920
istateOut =
         3
         3
         3
         2
         0
         0
         0
         3
         3
         3
clamdaOut =
    -0.0000
     0.0000
     0.0000
    -0.0000
    -4.3870
    -4.1056
    -5.4633
         0
         0
    -1.0000
miniz =
        628
minz =
        758
ninf =
         0
sinf =
         0
obj =
    5.1265e+03
user =
         0
lwsavOut =
         1

```

```

1
1
1
1
1
1
1
1
1
1
1
0
1
1
0
0
0
0
0
0
0
0
0
0
iwsavOut =
    array elided
rwsavOut =
    array elided
ifail =
    0

```

**Note:** the remainder of this document is intended for more advanced users. Section 10 contains a detailed description of the algorithm which may be needed in order to understand Sections 11 and 12. Section 11 describes the optional parameters which may be set by calls to e04uj. Section 12 describes the quantities which can be requested to monitor the course of the computation.

## 10 Algorithmic Details

This section contains a detailed description of the method used by e04ug.

### 10.1 Overview

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

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

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

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

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

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

A point  $x$  is a *first-order Kuhn–Karush–Tucker (KKT) point* for (1) (see Powell 1974) if the following conditions hold:

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

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

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

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

An equivalent statement of the condition (4) is

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

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

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

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

The basic structure of e04ug involves *major* and *minor* iterations. The major iterations generate a sequence of iterates  $\{x_k\}$  that satisfy the linear constraints and converge to a point  $x^*$  that satisfies the first-order KKT optimality conditions. At each iterate a QP subproblem is used to generate a search direction towards the next iterate ( $x_{k+1}$ ). The constraints of the subproblem are formed from the linear constraints  $Gx - s_L = 0$  and the nonlinear constraint linearization

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

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

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

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

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

then the QP subproblem can be written as

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

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

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

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

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

where the *basis matrix*  $B$  is square and nonsingular. The elements of  $x_B$ ,  $x_S$  and  $x_N$  are called the *basic*, *superbasic* and *nonbasic* variables respectively; they are a permutation of the elements of  $x$  and  $s$ . At a QP solution, the basic and superbasic variables will lie somewhere between their bounds, while the nonbasic variables will be equal to one of their upper or lower bounds. At each minor iteration,  $x_S$  is regarded as a set of independent variables that are free to move in any desired

direction, namely one that will improve the value of the QP objective function  $q(x)$  or sum of infeasibilities (as appropriate). The basic variables are then adjusted in order to ensure that  $(x, s)$  continues to satisfy  $Ax - s = b$ . The number of superbasic variables ( $n_S$  say) therefore indicates the number of degrees of freedom remaining after the constraints have been satisfied. In broad terms,  $n_S$  is a measure of *how nonlinear* the problem is. In particular,  $n_S$  will always be zero if there are no nonlinear constraints in (1) and  $f(x)$  is linear.

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

Associated with each of the  $m$  equality constraints  $Ax - s = b$  is a *dual variable*  $\pi_i$ . Similarly, each variable in  $(x, s)$  has an associated *reduced gradient*  $d_j$  (also known as a *reduced cost*). The reduced gradients for the variables  $x$  are the quantities  $g - A^T\pi$ , where  $g$  is the gradient of the QP objective function  $q(x)$ ; the reduced gradients for the slack variables  $s$  are the dual variables  $\pi$ . The QP subproblem (5) is optimal if  $d_j \geq 0$  for all nonbasic variables at their lower bounds,  $d_j \leq 0$  for all nonbasic variables at their upper bounds and  $d_j = 0$  for other variables (including superbasics). In practice, an *approximate* QP solution is found by slightly relaxing these conditions on  $d_j$  (see the description of the optional parameter **Minor Optimality Tolerance**).

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

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

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

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

produces a *sufficient decrease* in the merit function (6). When necessary, the penalties in  $D$  are increased by the minimum-norm perturbation that ensures descent for  $\mathcal{M}$  (see Gill *et al.* 1992). As in e04wd,  $s_N$  is adjusted to minimize the merit function as a function of  $s$  before the solution of the QP subproblem. Further details can be found in Eldersveld 1991 and Gill *et al.* 1986c.

## 10.2 Treatment of Constraint Infeasibilities

e04ug makes explicit allowance for infeasible constraints. Infeasible linear constraints are detected first by solving a problem of the form

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

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

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

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

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



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

where

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

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

## 11 Optional Parameters

Several optional parameters in e04ug define choices in the problem specification or the algorithm logic. In order to reduce the number of formal parameters of e04ug these optional parameters have associated *default values* that are appropriate for most problems. Therefore, you need only specify those optional parameters whose values are to be different from their default values.

The remainder of this section can be skipped if you wish to use the default values for *all* optional parameters. A complete list of optional parameters and their default values is given in Section 11.1.

Optional parameters may be specified by calling e04uj before a call to e04ug.

e04uj can be called to supply options directly, one call being necessary for each optional parameter. For example,

```
[lwsav, iwsav, rwsav, inform] = e04uj('Print Level = 5', lwsav, iwsav,
rwsav);
```

e04uj should be consulted for a full description of this method of supplying optional parameters.

All optional parameters not specified by you are set to their default values. Optional parameters specified by you are unaltered by e04ug (unless they define invalid values) and so remain in effect for subsequent calls to e04ug from the calling program (unless altered by you).

### 11.1 Optional Parameter Checklist and Default Values

The following list gives the valid options. For each option, we give the keyword, any essential optional qualifiers and the default value. A definition for each option can be found in Section 11.2. The minimum abbreviation of each keyword is underlined. If no characters of an optional qualifier are underlined, the qualifier may be omitted. The letters *i* and *r* denote integer and double values required with certain options. The default value of an option is used whenever the condition  $|i| \geq 100000000$  is satisfied.

Optional Parameters	Default Values
<u>Central Difference Interval</u>	Default = $\sqrt[3]{\text{Function Precision}}$
<u>Check Frequency</u>	Default = 60
<u>Crash Option</u>	Default = 0 or 3
<u>Crash Tolerance</u>	Default = 0.1
<u>Defaults</u>	
<u>Derivative Level</u>	Default = 3
<u>Derivative Linesearch</u>	Default
<u>Elastic Weight</u>	Default = 1.0 or 100.0
<u>Expand Frequency</u>	Default = 10000
<u>Factorization Frequency</u>	Default = 50 or 100
<u>Feasibility Tolerance</u>	See <u>Minor Feasibility Tolerance</u>
<u>Feasible Exit</u>	See <u>Infeasible Exit</u>
<u>Feasible Point</u>	See <u>Minimize</u>
<u>Forward Difference Interval</u>	Default = $\sqrt{\text{Function Precision}}$

<u>Function Precision</u>	Default = $\epsilon^{0.8}$
<u>Hessian Frequency</u>	Default = 99999999
<u>Hessian Full Memory</u>	Default = <b>Hessian Full Memory</b> if $\bar{n} < 75$
<u>Hessian Limited Memory</u>	Default = <b>Hessian Limited Memory</b> if $\bar{n} \geq 75$ . See <b>Hll Memory</b> .
<u>Hessian Updates</u>	Default = 20 or 99999999
<u>Infeasible Exit</u>	Default
<u>Infinite Bound Size</u>	Default = $10^{20}$
<u>Iteration Limit</u>	Default = 10000
<u>LU Density Tolerance</u>	Default = 0.6
<u>LU Factor Tolerance</u>	Default = 5.0 or 100.0
<u>LU Singularity Tolerance</u>	Default = $\epsilon^{0.67}$ . See <b>LU Density Tolerance</b> .
<u>LU Update Tolerance</u>	Default = 5.0 or 10.0. See <b>LU Factor Tolerance</b> .
<u>Linesearch Tolerance</u>	Default = 0.9
<u>List</u>	Default for e04ug = <b>List</b>
<u>Major Feasibility Tolerance</u>	Default = $\sqrt{\epsilon}$
<u>Major Iteration Limit</u>	Default = 1000
<u>Major Optimality Tolerance</u>	Default = $\sqrt{\epsilon}$
<u>Major Print Level</u>	Default for e04ug = 10
	Default for e04ug = 0
<u>Major Step Limit</u>	Default = 2.0
<u>Maximize</u>	See <b>Minimize</b>
<u>Minimize</u>	Default
<u>Minor Feasibility Tolerance</u>	Default = $\sqrt{\epsilon}$
<u>Minor Iteration Limit</u>	Default = 500
<u>Minor Optimality Tolerance</u>	Default = $\sqrt{\epsilon}$
<u>Minor Print Level</u>	Default = 0
<u>Monitoring File</u>	Default = -1
<u>Nolist</u>	Default for e04ug = <b>Nolist</b> . See <b>List</b> .
<u>Nonderivative Linesearch</u>	See <b>Derivative Linesearch</b>
<u>Optimality Tolerance</u>	See <b>Major Optimality Tolerance</b>
<u>Partial Price</u>	Default = 1 or 10
<u>Pivot Tolerance</u>	Default = $\epsilon^{0.67}$
<u>Print Level</u>	See <b>Major Print Level</b>
<u>Scale Option</u>	Default = 1 or 2
<u>Scale Tolerance</u>	Default = 0.9
<u>Start Constraint Check At Column</u>	Default = 1. See <b>Start Objective Check At Column</b> .
<u>Start Objective Check At Column</u>	Default = 1
<u>Stop Constraint Check At Column</u>	Default = $n_1''$ . See <b>Start Objective Check At Column</b> .
<u>Stop Objective Check At Column</u>	Default = $n_1'$ . See <b>Start Objective Check At Column</b> .
<u>Superbasics Limit</u>	Default = $\min(500, \bar{n} + 1)$
<u>Unbounded Objective</u>	Default = $10^{15}$
<u>Unbounded Step Size</u>	Default = $\max(\text{bigbnd}, 10^{20})$ . See <b>Unbounded Ob.</b>
<u>Verify Level</u>	Default = 0
<u>Violation Limit</u>	Default = 10.0

## 11.2 Description of the Optional Parameters

Central Difference Interval  $r$  Default =  $\sqrt[3]{\text{Function Precision}}$

Note that this option does not apply when **Derivative Level** = 3.

The value of  $r$  is used near an optimal solution in order to obtain more accurate (but more expensive) estimates of gradients. This requires twice as many function evaluations as compared to using forward differences (see optional parameter **Forward Difference Interval**). The interval used

for the  $j$ th variable is  $h_j = r(1 + |x_j|)$ . The resulting gradient estimates should be accurate to  $O(r^2)$ , unless the functions are badly scaled. The switch to central differences is indicated by  $c$  at the end of each line of intermediate printout produced by the major iterations (see Section 8.1). See Gill *et al.* 1981 for a discussion of the accuracy in finite difference approximations.

If  $r \leq 0$ , the default value is used.

### Check Frequency

 $i$ 

Default = 60

Every  $i$ th minor iteration after the most recent basis factorization, a numerical test is made to see if the current solution  $(x, s)$  satisfies the general linear constraints (including any linearized nonlinear constraints). The constraints are of the form  $Ax - s = b$ , where  $s$  is the set of slack variables. If the largest element of the residual vector  $r = b - Ax + s$  is judged to be too large, the current basis is refactorized and the basic variables recomputed to satisfy the general constraints more accurately.

If  $i < 0$ , the default value is used. If  $i = 0$ , the value  $i = 99999999$  is used and effectively no checks are made.

### Crash Option

 $i$ 

Default = 0 or 3

The default value of  $i$  is 0 if there are any nonlinear constraints and 3 otherwise. Note that this option does not apply when **start** = 'W' (see Section 5).

If **start** = 'C', an internal Crash procedure is used to select an initial basis from various rows and columns of the constraint matrix  $(A \ -I)$ . The value of  $i$  determines which rows and columns of  $A$  are initially eligible for the basis and how many times the Crash procedure is called. Columns of  $-I$  are used to pad the basis where necessary. The possible choices for  $i$  are the following.

 $i$ 

#### Meaning

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

If  $i < 0$  or  $i > 3$ , the default value is used.

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

### Crash Tolerance

 $r$ 

Default = 0.1

The value  $r$  ( $0 \leq r < 1$ ) allows the Crash procedure to ignore certain 'small' nonzero elements in the columns of  $A$  while searching for a triangular basis. If  $a_{\max}$  is the largest element in the  $j$ th column, other nonzeros  $a_{ij}$  in the column are ignored if  $|a_{ij}| \leq a_{\max} \times r$ .

When  $r > 0$ , the basis obtained by the Crash procedure may not be strictly triangular, but it is likely to be nonsingular and almost triangular. The intention is to obtain a starting basis containing more columns of  $A$  and fewer (arbitrary) slacks. A feasible solution may be reached earlier on some problems.

If  $r < 0$  or  $r \geq 1$ , the default value is used.

**Defaults**

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

**Derivative Level** $i$ 

Default = 3

This parameter indicates which nonlinear function gradients are provided in user-supplied (sub)programs **objfun** and **confun**. The possible choices for  $i$  are the following.

 $i$ **Meaning**

- 3 All elements of the objective gradient and the constraint Jacobian are provided.
- 2 All elements of the constraint Jacobian are provided, but some (or all) elements of the objective gradient are not specified.
- 1 All elements of the objective gradient are provided, but some (or all) elements of the constraint Jacobian are not specified.
- 0 Some (or all) elements of both the objective gradient and the constraint Jacobian are not specified.

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

If  $i = 0$  or  $2$ , e04ug will *estimate* the unspecified elements of the objective gradient, using finite differences. This may simplify the coding of (sub)program **objfun**. However, the computation of finite difference approximations usually increases the total run-time substantially (since a call to **objfun** is required for each unspecified element) and there is less assurance that an acceptable solution will be found.

If  $i = 0$  or  $1$ , e04ug will approximate unspecified elements of the constraint Jacobian. For each column of the Jacobian, one call to (sub)program **confun** is needed to estimate all unspecified elements in that column (if any). For example, if the sparsity pattern of the Jacobian has the form

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

where ‘\*’ indicates an element provided by you and ‘?’ indicates an unspecified element, e04ug will call **confun** twice: once to estimate the missing element in column 2 and again to estimate the two missing elements in column 3. (Since columns 1 and 4 are known, they require no calls to **confun**.)

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

If  $i < 0$  or  $i > 3$ , the default value is used.

**Derivative Linesearch**

Default

**Nonderivative Linesearch**

At each major iteration, a linesearch is used to improve the value of the Lagrangian merit function (6). The default linesearch uses safeguarded cubic interpolation and requires both function and gradient values in order to compute estimates of the step  $\alpha_k$ . If some analytic derivatives are not provided or optional parameter **Nonderivative Linesearch** is specified, a linesearch based upon safeguarded quadratic interpolation (which does not require the evaluation or approximation of any gradients) is used instead.

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

If optional parameter **Nonderivative Linesearch** is selected, e04ug signals the evaluation of the linesearch by calling the user-supplied (sub)programs **objfun** and **confun** with **mode** = 0. Once the

linesearch is complete, the nonlinear functions are re-evaluated with **mode** = 2. If the potential savings offered by a nonderivative linesearch are to be fully realized, it is essential that **objfun** and **confun** be coded so that no derivatives are computed when **mode** = 0.

### Elastic Weight

 $r$ 

Default = 1.0 or 100.0

The default value of  $r$  is 100.0 if there are any nonlinear constraints and 1.0 otherwise.

This option defines the initial weight  $\gamma$  associated with problem (8).

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

Thereafter,  $\gamma$  is increased (subject to a maximum allowable value) at any point that is optimal for problem (8), but not feasible for problem (1). After the  $p$ th increase,  $\gamma = r \times 10^p \times (1 + \|g(x_{k_1})\|_2)$ , where  $x_{k_1}$  is the iterate at which  $\gamma$  was first needed.

If  $r < 0$ , the default value is used.

### Expand Frequency

 $i$ 

Default = 10000

This option is part of the EXPAND anti-cycling procedure due to Gill *et al.* 1989, which is designed to make progress even on highly degenerate problems.

For linear models, the strategy is to force a positive step at every iteration, at the expense of violating the constraints by a small amount. Suppose that the value of optional parameter **Minor Feasibility Tolerance** is  $\delta$ . Over a period of  $i$  iterations, the feasibility tolerance actually used by e04ug (i.e., the *working* feasibility tolerance) increases from  $0.5\delta$  to  $\delta$  (in steps of  $0.5\delta/i$ ).

For nonlinear models, the same procedure is used for iterations in which there is only one superbasic variable. (Cycling can 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  $i$  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 optional parameter **Pivot Tolerance**).

If  $i < 0$ , the default value is used. If  $i = 0$ , the value  $i = 99999999$  is used and effectively no anti-cycling procedure is invoked.

### Factorization Frequency

 $i$ 

Default = 50 or 100

The default value of  $i$  is 50 if there are any nonlinear constraints and 100 otherwise.

If  $i > 0$ , at most  $i$  basis changes will occur between factorizations of the basis matrix.

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

When the objective function is nonlinear, fewer basis updates will occur as the solution is approached. The number of iterations between basis factorizations will therefore increase. During these iterations a test is made regularly according to the value of optional parameter **Check Frequency** to ensure that the general constraints are satisfied. If necessary, the basis will be refactored before the limit of  $i$  updates is reached.

If  $i \leq 0$ , the default value is used.

### Infeasible Exit

Default

### Feasible Exit

Note that this option is ignored if the value of optional parameter **Major Iteration Limit** is exceeded, or the linear constraints are infeasible.

If termination is about to occur at a point that does not satisfy the nonlinear constraints and optional parameter **Feasible Exit** is selected, this option requests that additional iterations be performed in order to find a feasible point (if any) for the nonlinear constraints. This involves solving a feasible point problem in which the objective function is omitted.

Otherwise, this option requests no additional iterations be performed.

### Minimize

Default

### Maximize

### Feasible Point

If optional parameter **Feasible Point** is selected, this option attempts to find a feasible point (if any) for the nonlinear constraints by omitting the objective function. It can also be used to check whether the nonlinear constraints are feasible.

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

### Forward Difference Interval

 $r$ Default =  $\sqrt{\text{Function Precision}}$ 

This option defines an interval used to estimate derivatives by forward differences in the following circumstances:

- (a) For verifying the objective and/or constraint gradients (see the description of the optional parameter **Verify Level**).
- (b) For estimating unspecified elements of the objective gradient and/or the constraint Jacobian.

A derivative with respect to  $x_j$  is estimated by perturbing that element of  $x$  to the value  $x_j + r(1 + |x_j|)$  and then evaluating  $f(x)$  and/or  $F(x)$  (as appropriate) at the perturbed point. The resulting gradient estimates should be accurate to  $O(r)$ , unless the functions are badly scaled. Judicious alteration of  $r$  may sometimes lead to greater accuracy. See Gill *et al.* 1981 for a discussion of the accuracy in finite difference approximations.

If  $r \leq 0$ , the default value is used.

### Function Precision

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

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

Ideally the functions  $f(x)$  or  $F_i(x)$  should have magnitude of order 1. If all functions are substantially *less* than 1 in magnitude,  $\epsilon_r$  should be the *absolute* precision. For example, if  $f(x)$  (or  $F_i(x)$ ) is computed as  $1.23456789 \times 10^{-4}$  for some relevant  $x$  and the first 6 significant digits are known to be correct then the appropriate value for  $\epsilon_r$  would be  $10^{-10}$ .

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

In some cases the function values will be the result of extensive computation, possibly involving an iterative procedure that can provide few digits of precision at reasonable cost. Specifying an appropriate value of  $r$  may therefore lead to savings, by allowing the linesearch procedure to terminate when the difference between function values along the search direction becomes as small as the absolute error in the values.

If  $r < \epsilon$  or  $r \geq 1$ , the default value is used.

**Hessian Frequency**  $i$  Default = 99999999

This option forces the approximate Hessian formed from  $i$  BFGS updates to be reset to the identity matrix upon completion of a major iteration. It is intended to be used in conjunction with optional parameter **Hessian Full Memory**.

If  $i \leq 0$ , the default value is used and effectively no resets occur.

**Hessian Full Memory** Default = **Hessian Full Memory** if  $\bar{n} < 75$   
**Hessian Limited Memory** Default = **Hessian Limited Memory** if  $\bar{n} \geq 75$

These options specify the method for storing and updating the quasi-Newton approximation to the Hessian of the Lagrangian function.

If **Hessian Full Memory** is specified, the approximate Hessian is treated as a dense matrix and BFGS quasi-Newton updates are applied explicitly. This is most efficient when the total number of nonlinear variables is not too large (say,  $\bar{n} < 75$ ). In this case, the storage requirement is fixed and you can expect 1-step Q-superlinear convergence to the solution.

**Hessian Limited Memory** should only be specified when  $\bar{n}$  is very large. In this case a limited memory procedure is used to update a diagonal Hessian approximation  $H_r$  a limited number of times. (Updates are accumulated as a list of vector pairs. They are discarded at regular intervals after  $H_r$  has been reset to their diagonal.)

Note that if **Hessian Frequency** = 20 is used in conjunction with **Hessian Full Memory**, the effect will be similar to using **Hessian Limited Memory** in conjunction with **Hessian Updates** = 20, except that the latter will retain the current diagonal during resets.

**Hessian Updates**  $i$  Default = 20 or 99999999

The default value of  $i$  is 20 when **Hessian Limited Memory** is in effect and 99999999 when **Hessian Full Memory** is in effect, in which case no updates are performed.

If **Hessian Limited Memory** is selected, this option defines the maximum number of pairs of Hessian update vectors that are to be used to define the quasi-Newton approximate Hessian. Once the limit of  $i$  updates is reached, all but the diagonal elements of the accumulated updates are discarded and the process starts again. Broadly speaking, the more updates that are stored, the better the quality of the approximate Hessian. On the other hand, the more vectors that are stored, the greater the cost of each QP iteration.

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

If  $i < 0$ , the default value is used.

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

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

If  $r \leq 0$ , the default value is used.

**Iteration Limit**  $i$  Default = 10000

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

If  $i < 0$ , the default value is used.

**Linesearch Tolerance**  $r$  Default = 0.9

This option controls the accuracy with which a step length will be located along the direction of search at each iteration. At the start of each linesearch a target directional derivative for the

Lagrangian merit function is identified. The value of  $r$  therefore determines the accuracy to which this target value is approximated.

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

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

If the nonlinear functions are expensive to evaluate, a less accurate search may be appropriate. If **Derivative Level** = 3, try  $r = 0.99$ . (The number of major iterations required to solve the problem might increase, but the total number of function evaluations may decrease enough to compensate.)

If **Derivative Level** < 3, a moderately accurate search may be appropriate; try  $r = 0.5$ . Each search will (typically) require only 1 – 5 function values, but many function calls will then be needed to estimate the missing gradients for the next iteration.

If  $r < 0$  or  $r \geq 1$ , the default value is used.

**List**  
**Nolist**

Default for e04ug = **List**  
Default for e04ug = **Nolist**

Normally each optional parameter specification is printed as it is supplied. Optional parameter **Nolist** may be used to suppress the printing and optional parameter **List** may be used to restore printing.

**LU Density Tolerance**

$r_1$

Default = 0.6

**LU Singularity Tolerance**

$r_2$

Default =  $\epsilon^{0.67}$

If  $r_1 > 0$ ,  $r_1$  defines the density tolerance used during the  $LU$  factorization of the basis matrix. Columns of  $L$  and rows of  $U$  are formed one at a time and the remaining rows and columns of the basis are altered appropriately. At any stage, if the density of the remaining matrix exceeds  $r_1$ , the Markowitz strategy for choosing pivots is terminated. The remaining matrix is then factorized using a dense  $LU$  procedure. Increasing the value of  $r_1$  towards unity may give slightly sparser  $LU$  factors, with a slight increase in factorization time. If  $r_1 \leq 0$ , the default value is used.

If  $r_2 > 0$ ,  $r_2$  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  $|u_{jj}| \leq r_2$  or  $|u_{jj}| < r_2 \times \max_i |u_{ij}|$ , the  $j$ th column of the basis is replaced by the corresponding slack variable.

This is most likely to occur when **start** = 'W' (see Section 5), or at the start of a major iteration. If  $r_2 \leq 0$ , the default value is used.

In some cases, the Jacobian matrix may converge to values that make the basis exactly singular (e.g., a whole row of the Jacobian matrix could be zero at an optimal solution). Before exact singularity occurs, the basis could become very ill-conditioned and the optimization could progress very slowly (if at all). Setting  $r_2 = 0.00001$  (say) may therefore help cause a judicious change of basis in such situations.

**LU Factor Tolerance**

$r_1$

Default = 5.0 or 100.0

**LU Update Tolerance**

$r_2$

Default = 5.0 or 10.0

The default value of  $r_1$  is 5.0 if there are any nonlinear constraints and 100.0 otherwise. The default value of  $r_2$  is 5.0 if there are any nonlinear constraints and 10.0 otherwise.

If  $r_1 \geq 1$  and  $r_2 \geq 1$ , the values of  $r_1$  and  $r_2$  affect the stability and sparsity of the basis factorization  $B = LU$ , during refactorization and updating, respectively. The lower triangular matrix  $L$  is a product of matrices of the form

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

where the multipliers  $\mu$  satisfy  $|\mu| \leq r_i$ . Smaller values of  $r_i$  favour stability, while larger values favour sparsity. The default values of  $r_1$  and  $r_2$  usually strike a good compromise. For large and



relatively dense problems, setting  $r_1 = 10.0$  or  $5.0$  (say) may give a marked improvement in sparsity without impairing stability to a serious degree. Note that for problems involving band matrices, it may be necessary to reduce  $r_1$  and/or  $r_2$  in order to achieve stability.

If  $r_1 < 1$  or  $r_2 < 1$ , the appropriate default value is used.

### **Major Feasibility Tolerance**

 $r$ Default =  $\sqrt{\epsilon}$ 

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

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

$$rowerr = \max_i \frac{viol_i}{\|(x, s)\|} \leq r,$$

where  $viol_i$  is the violation of the  $i$ th nonlinear constraint.

If  $r \leq \epsilon$ , the default value is used.

### **Major Iteration Limit**

 $i$ 

Default = 1000

The value of  $i$  specifies the maximum number of major iterations allowed before termination. It is intended to guard against an excessive number of linearizations of the nonlinear constraints. Setting  $i = 0$  and **Major Print Level**  $> 0$  means that the objective and constraint gradients will be checked if **Verify Level**  $> 0$  and the workspace needed to start solving the problem will be computed and printed, but no iterations will be performed.

If  $i < 0$ , the default value is used.

### **Major Optimality Tolerance**

 $r$ Default =  $\sqrt{\epsilon}$ 

#### **Optimality Tolerance**

 $r$ 

This option specifies the final accuracy of the dual variables. If e04ug terminates with **ifail** = 0, a primal and dual solution  $(x, s, \pi)$  will have been computed such that

$$maxgap = \max_j \frac{gap_j}{\|\pi\|} \leq r,$$

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

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

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

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

If  $r \leq 0$ , the default value is used.

### **Major Print Level**

 $i$ 

Default for e04ug = 10

Default for e04ug = 0

#### **Print Level**

The value of  $i$  controls the amount of printout produced by the major iterations of e04ug, as indicated below. A detailed description of the printed output is given in Section 8.1 (summary

output at each major iteration and the final solution) and Section 12 (monitoring information at each major iteration). (See also the description of **Minor Print Level**.)

The following printout is sent to the current advisory message unit (as defined by x04ab):

<i>i</i>	Output
0	No output.
1	The final solution only.
5	One line of summary output ( < 80 characters; see Section 8.1) for each major iteration (no printout of the final solution).
≥ 10	The final solution and one line of summary output for each major iteration.

The following printout is sent to the logical unit number defined by the optional parameter **Monitoring File**:

<i>i</i>	Output
0	No output.
1	The final solution only.
5	One long line of output ( < 120 characters; see Section 12) for each major iteration (no printout of the final solution).
≥ 10	The final solution and one long line of output for each major iteration.
≥ 20	The final solution, one long line of output for each major iteration, matrix statistics (initial status of rows and columns, number of elements, density, biggest and smallest elements, etc.), details of the scale factors resulting from the scaling procedure (if <b>Scale Option</b> = 1 or 2), basis factorization statistics and details of the initial basis resulting from the Crash procedure (if <b>start</b> = 'C'; see Section 5).

If **Major Print Level** ≥ 5 and the unit number defined by the optional parameter **Monitoring File** is the same as that defined by x04ab then the summary output for each major iteration is suppressed.

### Major Step Limit

*r*

Default = 2.0

If  $r > 0$ ,  $r$  limits the change in  $x$  during a linesearch. It applies to all nonlinear problems once a 'feasible solution' or 'feasible subproblem' has been found.

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

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

$$\bar{\beta} = \frac{r(1 + \|x\|_2)}{\|p\|_2},$$

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

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

If  $r \leq 0$ , the default value is used.

### Minor Feasibility Tolerance Feasibility Tolerance

*r*Default =  $\sqrt{\epsilon}$ *r*

This option attempts to ensure that all variables eventually satisfy their upper and lower bounds to within the tolerance  $r$ . Since this includes slack variables, general linear constraints should also be satisfied to within  $r$ . Note that feasibility with respect to nonlinear constraints is judged by the value of optional parameter **Major Feasibility Tolerance** and not by  $r$ .

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

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

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

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

If  $r \leq \epsilon$ , the default value is used.

### **Minor Iteration Limit**

$i$

Default = 500

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

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

If  $i \leq 0$ , the default value is used.

### **Minor Optimality Tolerance**

$r$

Default =  $\sqrt{\epsilon}$

This option is used to judge optimality for each QP subproblem. Let the QP reduced gradients be  $d_j = g_j - \pi^T a_j$ , where  $g_j$  is the  $j$ th element of the QP gradient,  $a_j$  is the associated column of the QP constraint matrix and  $\pi$  is the set of QP dual variables.

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

$$\frac{d_j}{\|\pi\|} \geq -r \quad \text{or} \quad \frac{d_j}{\|\pi\|} \leq r$$

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

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

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

If  $r \leq 0$ , the default value is used.

**Minor Print Level** $i$ 

Default = 0

The value of  $i$  controls the amount of printout produced by the minor iterations of e04ug (i.e., the iterations of the quadratic programming algorithm), as indicated below. A detailed description of the printed output is given in Section 8.2 (summary output at each minor iteration) and Section 12 (monitoring information at each minor iteration). (See also the description of the optional parameter **Major Print Level**.)

The following printout is sent to the current advisory message unit (as defined by x04ab):

 $i$ **Output**

- 0 No output.
- $\geq 1$  One line of summary output (< 80 characters; see Section 8.2) for each minor iteration.

The following printout is sent to the logical unit number defined by the optional parameter **Monitoring File**:

 $i$ **Output**

- 0 No output.
- $\geq 1$  One long line of output (< 120 characters; see Section 12) for each minor iteration.

If **Minor Print Level**  $\geq 1$  and the unit number defined by the optional parameter **Monitoring File** is the same as that defined by x04ab then the summary output for each minor iteration is suppressed.

**Monitoring File** $i$ 

Default = -1

If  $i \geq 0$  and **Major Print Level**  $\geq 5$  or  $i \geq 0$  and **Minor Print Level**  $\geq 1$  then monitoring information is produced by e04ug at every iteration is sent to a file with logical unit number  $i$ . If  $i < 0$  and/or **Major Print Level**  $< 5$  and **Minor Print Level**  $< 1$  then no monitoring information is produced.

**Partial Price** $i$ 

Default = 1 or 10

The default value of  $i$  is 1 if there are any nonlinear constraints and 10 otherwise.

This option is recommended for large 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 become superbasic). The possible choices for  $i$  are the following.

 $i$ **Meaning**

- 1 All columns of the constraint matrix ( $A \ -I$ ) are searched.
- $\geq 2$  Both  $A$  and  $I$  are partitioned to give  $i$  roughly equal segments  $A_j, I_j$ , for  $j = 1, 2, \dots, p$  (modulo  $p$ ). If the previous pricing search was successful on  $A_j, I_j$ , the next search begins on the segments  $A_{j+1}, I_{j+1}$ . If a reduced gradient is found that is larger than some dynamic tolerance, the variable with the largest such reduced gradient (of appropriate sign) is selected to enter the basis. If nothing is found, the search continues on the next segments  $A_{j+2}, I_{j+2}$  and so on.

If  $i \leq 0$ , the default value is used.

**Pivot Tolerance** $r$ Default =  $\epsilon^{0.67}$ 

If  $r > 0$ ,  $r$  is used during the solution of QP subproblems to prevent columns entering the basis if they would cause the basis to become almost singular.

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

It is common in practice for two (or more) variables to reach a bound at essentially the same time. In such cases, the **Minor Feasibility Tolerance** provides some freedom to maximize the pivot element and thereby improve numerical stability. Excessively *small* values of **Minor Feasibility**

**Tolerance** should therefore not be specified. To a lesser extent, the **Expand Frequency** also provides some freedom to maximize the pivot element. Excessively *large* values of **Expand Frequency** should therefore not be specified.

If  $r \leq 0$ , the default value is used.

### Scale Option

 $i$ 

Default = 1 or 2

The default value of  $i$  is 1 if there are any nonlinear constraints and 2 otherwise.

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

 $i$ 

### Meaning

- 0 No scaling is performed. This is recommended if it is known that the elements of  $x$  and the constraint matrix  $A$  (along with its Jacobian) never become large (say,  $> 1000$ ).
- 1 All linear constraints and variables are scaled. This may improve the overall efficiency of the function on some problems.
- 2 All constraints and variables are scaled. Also, an additional scaling is performed that takes into account columns of  $(A \ -I)$  that are fixed or have positive lower bounds or negative upper bounds.

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

If  $i < 0$  or  $i > 2$ , the default value is used.

### Scale Tolerance

 $r$ 

Default = 0.9

Note that this option does not apply when **Scale Option** = 0.

The value  $r$  ( $0 < r < 1$ ) is used to control the number of scaling passes to be made through the constraint matrix  $A$ . At least 3 (and at most 10) passes will be made. More precisely, let  $a_p$  denote the largest column ratio (i.e.,  $\frac{\text{‘biggest’ element}}{\text{‘smallest’ element}}$  in some sense) after the  $p$ th scaling pass through  $A$ . The scaling procedure is terminated if  $a_p \geq a_{p-1} \times r$  for some  $p \geq 3$ . Thus, increasing the value of  $r$  from 0.9 to 0.99 (say) will probably increase the number of passes through  $A$ .

If  $r \leq 0$  or  $r \geq 1$ , the default value is used.

### Start Objective Check At Column

 $i_1$ 

Default = 1

### Stop Objective Check At Column

 $i_2$ Default =  $n'_1$ 

### Start Constraint Check At Column

 $i_3$ 

Default = 1

### Stop Constraint Check At Column

Default =  $n''_1$ 

These keywords take effect only if **Verify Level**  $> 0$ . They may be used to control the verification of gradient elements computed by (sub)program **objfun** and/or Jacobian elements computed by (sub)program **confun**. For example, if the first 30 elements of the objective gradient appeared to be correct in an earlier run, so that only element 31 remains questionable then it is reasonable to specify **Start Objective Check At Column** = 31. Similarly for columns of the Jacobian. If the first 30 variables occur nonlinearly in the constraints but the remaining variables are nonlinear only in the objective, then **objfun** must set the first 30 elements of the array **objgrd** to zero, but these hardly need to be verified. Again it is reasonable to specify **Start Objective Check At Column** = 31.

If  $i_2 \leq 0$  or  $i_2 > n'_1$ , the default value is used.

If  $i_1 \leq 0$  or  $i_1 > \min(n'_1, i_2)$ , the default value is used.

If  $i_4 \leq 0$  or  $i_4 > n_1''$ , the default value is used.

If  $i_3 \leq 0$  or  $i_3 > \min(n_1'', i_4)$ , the default value is used.

### **Superbasics Limit**

$i$

Default =  $\min(500, \bar{n} + 1)$

Note that this option does not apply to linear problems.

It places a limit on the storage allocated for superbasic variables. Ideally, the value of  $i$  should be set slightly larger than the ‘number of degrees of freedom’ expected at the solution.

For nonlinear problems, the number of degrees of freedom is often called the ‘number of independent variables’. Normally, the value of  $i$  need not be greater than  $\bar{n} + 1$ , but for many problems it may be considerably smaller. (This will save storage if  $\bar{n}$  is very large.)

If  $i \leq 0$ , the default value is used.

### **Unbounded Objective**

$r_1$

Default =  $10^{15}$

### **Unbounded Step Size**

$r_2$

Default =  $\max(\text{bigbnd}, 10^{20})$

These options are intended to detect unboundedness in nonlinear problems. During the linesearch, the objective function  $f$  is evaluated at points of the form  $x + \alpha p$ , where  $x$  and  $p$  are fixed and  $\alpha$  varies. If  $|f|$  exceeds  $r_1$  or  $\alpha$  exceeds  $r_2$ , the iterations are terminated and the function returns with **ifail** = 3.

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

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

If  $r_1 \leq 0$  or  $r_2 \leq 0$ , the appropriate default value is used.

### **Verify Level**

$i$

Default = 0

This option refers to finite difference checks on the gradient elements computed by the user-supplied (sub)programs **objfun** and **confun**. Gradients are verified at the first point that satisfies the linear constraints and the upper and lower bounds. Unspecified gradient elements are not checked and hence they result in no overhead. The possible choices for  $i$  are the following.

$i$	Meaning
-1	No checks are performed.
0	Only a ‘cheap’ test will be performed, requiring three calls to (sub)program <b>objfun</b> and two calls to (sub)program <b>confun</b> . Note that no checks are carried out if every column of the constraint gradients (Jacobian) contains a missing element.
1	Individual objective gradient elements will be checked using a reliable (but more expensive) test. If <b>Major Print Level</b> > 0, a key of the form OK or BAD? indicates whether or not each element appears to be correct.
2	Individual columns of the constraint gradients (Jacobian) will be checked using a reliable (but more expensive) test. If <b>Major Print Level</b> > 0, a key of the form OK or BAD? indicates whether or not each element appears to be correct.
3	Check both constraint and objective gradients (in that order) as described above for $i = 2$ and $i = 1$ respectively.

The value  $i = 3$  should be used whenever a new function function is being developed. The **Start** and **Stop** keywords may be used to limit the number of nonlinear variables to be checked.

If  $i < -1$  or  $i > 3$ , the default value is used.

### **Violation Limit**

$r$

Default = 10.0

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

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

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

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

If  $r \leq 0$ , the default value is used.

## 12 Description of Monitoring Information

This section describes the intermediate printout and final printout which constitutes the monitoring information produced by e04ug. (See also the description of the optional parameters **Monitoring File**, **Major Print Level** and **Minor Print Level**.) You can control the level of printed output.

When **Major Print Level**  $\geq 20$  and **Monitoring File**  $\geq 0$ , the following line of intermediate printout (< 120 characters) is produced at every major iteration on the unit number specified by optional parameter **Monitoring File**. Unless stated otherwise, the values of the quantities printed are those in effect *on completion* of the given iteration.

Major	is the major iteration count.
Minor	is the number of minor iterations required by the feasibility and optimality phases of the QP subproblem. Generally, Minor will be 1 in the later iterations, since theoretical analysis predicts that the correct active set will be identified near the solution (see Section 10).
Step	is the step $\alpha_k$ taken along the computed search direction. On reasonably well-behaved problems, the unit step (i.e., $\alpha_k = 1$ ) will be taken as the solution is approached.
nObj	is the number of times (sub)program <b>objfun</b> has been called to evaluate the nonlinear part of the objective function. Evaluations needed for the estimation of the gradients by finite differences are not included. nObj is printed as a guide to the amount of work required for the linesearch.
nCon	is the number of times (sub)program <b>confun</b> has been called to evaluate the nonlinear constraint functions (not printed if <b>ncnln</b> is zero).
Merit	is the value of the augmented Lagrangian merit function (6) at the current iterate. This function will decrease at each iteration unless it was necessary to increase the penalty parameters (see Section 8.1). As the solution is approached, Merit will converge to the value of the objective function at the solution.  In elastic mode (see Section 10.2), the merit function is a composite function involving the constraint violations weighted by the value of the optional parameter <b>Elastic Weight</b> .  If there are no nonlinear constraints present, this entry contains Objective, the value of the objective function $f(x)$ . In this case, $f(x)$ will decrease monotonically to its optimal value.
Feasibl	is the value of <i>rowerr</i> , the largest element of the scaled nonlinear constraint residual vector defined in the description of the optional parameter <b>Major Feasibility Tolerance</b> . The solution is regarded as ‘feasible’ if Feasibl is less than (or equal to) the optional parameter <b>Major Feasibility Tolerance</b> . Feasibl will be approximately zero in the neighbourhood of a solution.

	<p>If there are no nonlinear constraints present, all iterates are feasible and this entry is not printed.</p>
Optimal	<p>is the value of <i>maxgap</i>, the largest element of the maximum complementarity gap vector defined in the description of the optional parameter <b>Major Optimality Tolerance</b>. The Lagrange multipliers are regarded as ‘optimal’ if Optimal is less than (or equal to) the optional parameter <b>Major Optimality Tolerance</b>. Optimal will be approximately zero in the neighbourhood of a solution.</p>
nS	<p>is the current number of superbasic variables.</p>
Penalty	<p>is the Euclidean norm of the vector of penalty parameters used in the augmented Lagrangian merit function (not printed if <b>ncnln</b> is zero).</p>
LU	<p>is the number of nonzeros representing the basis factors <i>L</i> and <i>U</i> on completion of the QP subproblem.</p> <p>If there are nonlinear constraints present, the basis factorization <math>B = LU</math> is computed at the start of the first minor iteration. At this stage, <math>LU = \text{lenL} + \text{lenU}</math>, where <i>lenL</i> is the number of subdiagonal elements in the columns of a lower triangular matrix and <i>lenU</i> is the number of diagonal and superdiagonal elements in the rows of an upper triangular matrix. As columns of <i>B</i> are replaced during the minor iterations, the value of LU may fluctuate up or down (but in general will tend to increase). As the solution is approached and the number of minor iterations required to solve each QP subproblem decreases towards zero, LU will reflect the number of nonzeros in the <i>LU</i> factors at the start of each QP subproblem.</p> <p>If there are no nonlinear constraints present, refactorization is subject only to the value of the optional parameter <b>Factorization Frequency</b> and hence LU will tend to increase between factorizations.</p>
Swp	<p>is the number of columns of the basis matrix <i>B</i> that were swapped with columns of <i>S</i> in order to improve the condition number of <i>B</i> (not printed if <b>ncnln</b> is zero). The swaps are determined by an <i>LU</i> factorization of the rectangular matrix <math>B_S = (B \ S)^T</math>, with stability being favoured more than sparsity.</p>
Cond Hz	<p>is an estimate of the condition number of the reduced Hessian of the Lagrangian (not printed if <b>ncnln</b> and <b>nonln</b> are both zero). It is the square of the ratio between the largest and smallest diagonal elements of the upper triangular matrix <i>R</i>. This constitutes a lower bound on the condition number of the matrix <math>R^T R</math> that approximates the reduced Hessian. The larger this number, the more difficult the problem.</p>
PD	<p>is a two-letter indication of the status of the convergence tests involving the feasibility and optimality of the iterates defined in the descriptions of the optional parameters <b>Major Feasibility Tolerance</b> and <b>Major Optimality Tolerance</b>. Each letter is T if the test is satisfied and F otherwise. The tests indicate whether the values of <i>Feasibl</i> and <i>Optimal</i> are sufficiently small. For example, TF or TT is printed if there are no nonlinear constraints present (since all iterates are feasible). If either indicator is F when e04ug terminates with <b>ifail</b> = 0, you should check the solution carefully.</p>
M	<p>is printed if an extra evaluation of user-supplied (sub)programs <b>objfun</b> and <b>confun</b> was needed in order to define an acceptable positive-definite quasi-Newton update to the Hessian of the Lagrangian. This modification is only performed when there are nonlinear constraints present.</p>
m	<p>is printed if, in addition, it was also necessary to modify the update to include an augmented Lagrangian term.</p>



s	is printed if a self-scaled BFGS (Broyden–Fletcher–Goldfarb–Shanno) update was performed. This update is always used when the Hessian approximation is diagonal and hence always follows a Hessian reset.
S	is printed if, in addition, it was also necessary to modify the self-scaled update in order to maintain positive-definiteness.
n	is printed if no positive-definite BFGS update could be found, in which case the approximate Hessian is unchanged from the previous iteration.
r	is printed if the approximate Hessian was reset after 10 consecutive major iterations in which no BFGS update could be made. The diagonal elements of the approximate Hessian are retained if at least one update has been performed since the last reset. Otherwise, the approximate Hessian is reset to the identity matrix.
R	is printed if the approximate Hessian has been reset by discarding all but its diagonal elements. This reset will be forced periodically by the values of the optional parameters <b>Hessian Frequency</b> and <b>Hessian Updates</b> . However, it may also be necessary to reset an ill-conditioned Hessian from time to time.
l	is printed if the change in the norm of the variables was greater than the value defined by the optional parameter <b>Major Step Limit</b> . If this output occurs frequently during later iterations, it may be worthwhile increasing the value of <b>Major Step Limit</b> .
c	is printed if central differences have been used to compute the unknown elements of the objective and constraint gradients. A switch to central differences is made if either the linesearch gives a small step, or $x$ is close to being optimal. In some cases, it may be necessary to re-solve the QP subproblem with the central difference gradient and Jacobian.
u	is printed if the QP subproblem was unbounded.
t	is printed if the minor iterations were terminated after the number of iterations specified by the value of the optional parameter <b>Minor Iteration Limit</b> was reached.
i	is printed if the QP subproblem was infeasible when the function was not in elastic mode. This event triggers the start of nonlinear elastic mode, which remains in effect for all subsequent iterations. Once in elastic mode, the QP subproblems are associated with the elastic problem (8) (see Section 10.2). It is also printed if the minimizer of the elastic subproblem does not satisfy the linearized constraints when the function is already in elastic mode. (In this case, a feasible point for the usual QP subproblem may or may not exist.)
w	is printed if a weak solution of the QP subproblem was found.

When **Minor Print Level**  $\geq 1$  and **Monitoring File**  $\geq 0$ , the following line of intermediate printout ( $< 120$  characters) is produced at every minor iteration on the unit number specified by optional parameter **Monitoring File**. Unless stated otherwise, the values of the quantities printed are those in effect *on completion* of the given iteration.

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

Itn	is the iteration count.
pp	is the partial price indicator. The variable selected by the last pricing operation came from the 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.

+SBS	is the variable selected by the pricing operation to be added to the superbasic set.
-SBS	is the variable chosen to leave the superbasic set. It has become basic if the entry under -B is nonzero; otherwise it has become nonbasic.
-BS	is the variable removed from the basis (if any) to become nonbasic.
-B	is the variable removed from the basis (if any) to swap with a slack variable made superbasic by the latest pricing operation. The swap is done to ensure that there are no superbasic slacks.
Step	is the value of the step length $\alpha$ taken along the current search direction $p$ . The variables $x$ have just been changed to $x + \alpha p$ . If a variable is made superbasic during the current iteration (i.e., +SBS is positive), Step will be the step to the nearest bound. During the optimality phase, the step can be greater than unity only if the reduced Hessian is not positive-definite.
Pivot	is the $r$ th element of a vector $y$ satisfying $By = a_q$ whenever $a_q$ (the $q$ th column of the constraint matrix $(A \ -I)$ ) replaces the $r$ th column of the basis matrix $B$ . Wherever possible, Step is chosen so as to avoid extremely small values of Pivot (since they may cause the basis to be nearly singular). In extreme cases, it may be necessary to increase the value of the optional parameter <b>Pivot Tolerance</b> to exclude very small elements of $y$ from consideration during the computation of Step.
Ninf	is the number of infeasibilities. This will not increase unless the iterations are in elastic mode. Ninf will be zero during the optimality phase.
Sinf/Objective	is the value of the current objective function. If $x$ is infeasible, Sinf gives the value of the sum of infeasibilities at the start of the current iteration. It will usually decrease at each nonzero value of Step, but may occasionally increase if the value of Ninf decreases by a factor of 2 or more. However, in elastic mode this entry gives the value of the composite objective function (9), which will decrease monotonically at each iteration. If $x$ is feasible, Objective is the value of the current QP objective function.
L	is the number of nonzeros in the basis factor $L$ . Immediately after a basis factorization $B = LU$ , this entry contains lenL. Further nonzeros are added to L when various columns of $B$ are later replaced. (Thus, L increases monotonically.)
U	is the number of nonzeros in the basis factor $U$ . Immediately after a basis factorization $B = LU$ , this entry contains lenU. As columns of $B$ are replaced, the matrix $U$ is maintained explicitly (in sparse form). The value of U may fluctuate up or down; in general, it will tend to increase.
Ncp	is the number of compressions required to recover workspace in the data structure for $U$ . This includes the number of compressions needed during the previous basis factorization. Normally, Ncp should increase very slowly. If it does not, increase <b>leniz</b> and <b>lenz</b> by at least $L + U$ and rerun e04ug (possibly using <b>start</b> = 'W'; see Section 5).

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

Norm rg	is the Euclidean norm of the reduced gradient of the QP objective function. During the optimality phase, this norm will be approximately zero after a unit step.
nS	is the current number of superbasic variables.
Cond Hz	is an estimate of the condition number of the reduced Hessian of the Lagrangian (not printed if <b>ncnl</b> and <b>nonln</b> are both zero). It is the square of the ratio between the largest and smallest diagonal elements of the upper triangular matrix $R$ . This constitutes a lower bound on the condition number

of the matrix  $R^T R$  that approximates the reduced Hessian. The larger this number, the more difficult the problem.

When **Major Print Level**  $\geq 20$  and **Monitoring File**  $\geq 0$ , the following lines of intermediate printout (< 120 characters) are produced on the unit number specified by optional parameter **Monitoring File** whenever the matrix  $B$  or  $B_S = (B \quad S)^T$  is factorized before solving the next QP subproblem. Gaussian elimination is used to compute a sparse  $LU$  factorization of  $B$  or  $B_S$ , where  $PLP^T$  is a lower triangular matrix and  $PUQ$  is an upper triangular matrix for some permutation matrices  $P$  and  $Q$ . The factorization is stabilized in the manner described under the optional parameter **LU Factor Tolerance** (default value = 5.0 or 100.0).

Note that  $B_S$  may be factorized at the beginning of just some of the major iterations. It is immediately followed by a factorization of  $B$  itself.

Factorize	is the factorization count.
Iteration	is the iteration count.
Nonlinear	is the number of nonlinear variables in the current basis $B$ (not printed if $B_S$ is factorized).
Linear	is the number of linear variables in $B$ (not printed if $B_S$ is factorized).
Slacks	is the number of slack variables in $B$ (not printed if $B_S$ is factorized).
Elms	is the number of nonzeros in $B$ (not printed if $B_S$ is factorized).
Density	is the percentage nonzero density of $B$ (not printed if $B_S$ is factorized). More precisely, $\text{Density} = 100 \times \text{Elms} / (\text{Nonlinear} + \text{Linear} + \text{Slacks})^2$ .
Compressns	is the number of times the data structure holding the partially factorized matrix needed to be compressed, in order to recover unused workspace. Ideally, it should be zero. If it is more than 3 or 4, increase <b>leniz</b> and <b>lenz</b> and rerun e04ug (possibly using <b>start</b> = 'W'; see Section 5).
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 $m = U_t + L_t + \text{bp}$ .
Ut	is the number of triangular rows of $B$ at the top of $U$ .
d1	is the number of columns remaining when the density of the basis matrix being factorized reached 0.3.
Lmax	is the maximum subdiagonal element in the columns of $L$ . This will not exceed the value of the optional parameter <b>LU Factor Tolerance</b> .
Bmax	is the maximum nonzero element in $B$ (not printed if $B_S$ is factorized).
BSmax	is the maximum nonzero element in $B_S$ (not printed if $B$ is factorized).
Umax	is the maximum nonzero element in $U$ , excluding elements of $B$ that remain in $U$ unchanged. (For example, if a slack variable is in the basis, the corresponding row of $B$ will become a row of $U$ without modification. Elements in such rows will not contribute to $U_{\max}$ . If the basis is strictly

triangular then *none* 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 parameter **LU Factor Tolerance** to some value nearer unity.

$U_{\max}$  is not printed if  $B_S$  is factorized.

$U_{\min}$	is the magnitude of the smallest diagonal element of $PUQ$ .
Growth	is the value of the ratio $U_{\max}/B_{\max}$ , which should not be too large.  Providing $L_{\max}$ is not large (say, $< 10.0$ ), the ratio $\max(B_{\max}, U_{\max})/U_{\min}$ is an estimate of the condition number of $B$ . If this number is extremely large, the basis is nearly singular and some numerical difficulties might occur. (However, an effort is made to avoid near-singularity by using slacks to replace columns of $B$ that would have made $U_{\min}$ extremely small and the modified basis is refactorized.)
$L_t$	is the number of triangular columns of $B$ at the left of $L$ .
$bp$	is the size of the ‘bump’ or block to be factorized nontrivially after the triangular rows and columns of $B$ have been removed.
$d2$	is the number of columns remaining when the density of the basis matrix being factorized has reached 0.6.

When **Major Print Level**  $\geq 20$ , **Monitoring File**  $\geq 0$  and **Crash Option**  $> 0$  (default value = 0 or 3), the following lines of intermediate printout ( $< 80$  characters) are produced on the unit number specified by optional parameter **Monitoring File** whenever **start** = ‘C’ (see Section 5). They refer to the number of columns selected by the Crash procedure during each of several passes through  $A$  while searching for a triangular basis matrix.

Slacks	is the number of slacks selected initially.
Free cols	is the number of free columns in the basis, including those whose bounds are rather far apart.
Preferred	is the number of ‘preferred’ columns in the basis (i.e., $\mathbf{istate}(j) = 3$ for some $j \leq n$ ). It will be a subset of the columns for which $\mathbf{istate}(j) = 3$ was specified.
Unit	is the number of unit columns in the basis.
Double	is the number of columns in the basis containing two nonzeros.
Triangle	is the number of triangular columns in the basis with three (or more) nonzeros.
Pad	is the number of slacks used to pad the basis (to make it a nonsingular triangle).

When **Major Print Level** = 1 or  $\geq 10$  and **Monitoring File**  $\geq 0$ , the following lines of final printout ( $< 120$  characters) are produced on the unit number specified by optional parameter **Monitoring File**.

Let  $x_j$  denote the  $j$ th ‘column variable’, for  $j = 1, 2, \dots, n$ . We assume that a typical variable  $x_j$  has bounds  $\alpha \leq x_j \leq \beta$ .

The following describes the printout for each column (or variable). A full stop (.) is printed for any numerical value that is zero.

Number	is the column number $j$ . (This is used internally to refer to $x_j$ in the intermediate output.)
Column	gives the name of $x_j$ .
State	gives the state of $x_j$ relative to the bounds $\alpha$ and $\beta$ .

The various possible states are as follows:

- LL  $x_j$  is nonbasic at its lower limit,  $\alpha$ .
- UL  $x_j$  is nonbasic at its upper limit,  $\beta$ .
- EQ  $x_j$  is nonbasic and fixed at the value  $\alpha = \beta$ .
- FR  $x_j$  is nonbasic at some value strictly between its bounds:  $\alpha < x_j < \beta$ .
- BS  $x_j$  is basic. Usually  $\alpha < x_j < \beta$ .

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

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

Activity	is the value of $x_j$ at the final iterate.
Obj Gradient	is the value of $g_j$ at the final iterate. (If any $x_j$ is infeasible, $g_j$ is the gradient of the sum of infeasibilities.)
Lower Bound	is the lower bound specified for the variable. None indicates that $\mathbf{bl}(j) \leq -bigbnd$ .
Upper Bound	is the upper bound specified for the variable. None indicates that $\mathbf{bu}(j) \geq bigbnd$ .
Reduced Gradnt	is the value of $d_j$ at the final iterate.
$m + j$	is the value of $m + j$ .

General linear constraints take the form  $l \leq Ax \leq u$ . The  $i$ th constraint is therefore of the form  $\alpha \leq a_i^T x \leq \beta$  and the value of  $a_i^T x$  is called the *row activity*. Internally, the linear constraints take the form  $Ax - s = 0$ , where the slack variables  $s$  should satisfy the bounds  $l \leq s \leq u$ . For the  $i$ th ‘row’, it is the slack variable  $s_i$  that is directly available and it is sometimes convenient to refer to its state. Slacks may be basic or nonbasic (but not superbasic).

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

The following describes the printout for each row (or constraint). A full stop (.) is printed for any numerical value that is zero.

Number	is the value of $n + i$ . (This is used internally to refer to $s_i$ in the intermediate output.)
Row	gives the name of the $i$ th row.
State	gives the state of the $i$ th row relative to the bounds $\alpha$ and $\beta$ .

The various possible states are as follows:

- LL The row is at its lower limit,  $\alpha$ .
- UL The row is at its upper limit,  $\beta$ .
- EQ The limits are the same ( $\alpha = \beta$ ).
- BS The constraint is not binding.  $s_i$  is basic.

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

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

Activity	is the value of $a_i^T x$ (or $F_i(x) + a_i^T x$ for nonlinear rows) at the final iterate.
Slack Activity	is the value by which the row differs from its nearest bound. (For the free row (if any), it is set to Activity.)
Lower Bound	is $\alpha$ , the lower bound specified for the $i$ th row. None indicates that $\mathbf{bl}(n + i) \leq -\mathbf{bigbnd}$ .
Upper Bound	is $\beta$ , the upper bound specified for the $i$ th row. None indicates that $\mathbf{bu}(n + i) \geq \mathbf{bigbnd}$ .
Dual Activity	is the value of the dual variable $\pi_i$ .
i	gives the index $i$ of the $i$ th row.

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