

NAG Library Function Document

nag_glopt_nlp_multistart_sqp_lsq (e05usc)

1 Purpose

nag_glopt_nlp_multistart_sqp_lsq (e05usc) is designed to find the global minimum of an arbitrary smooth sum of squares function subject to constraints (which may include simple bounds on the variables, linear constraints and smooth nonlinear constraints) by generating a number of different starting points and performing a local search from each using sequential quadratic programming.

2 Specification

```
#include <nag.h>
#include <nage05.h>

void nag_glopt_nlp_multistart_sqp_lsq (Integer m, Integer n, Integer nclin,
    Integer ncnln, const double a[], Integer pda, const double bl[],
    const double bu[], const double y[],

    void (*confun)(Integer *mode, Integer ncnln, Integer n, Integer pdcjsl,
        const Integer needc[], const double x[], double c[], double cjsl[],
        Integer nstate, Nag_Comm *comm),

    void (*objfun)(Integer *mode, Integer m, Integer n, Integer pdfjsl,
        Integer needfi, const double x[], double f[], double fjsl[],
        Integer nstate, Nag_Comm *comm),

    Integer npts, double x[], Integer pdx,

    void (*start)(Integer npts, double quas[], Integer n,
        Nag_Boolean repeat1, const double bl[], const double bu[],
        Nag_Comm *comm, Integer *mode),

    Nag_Boolean repeat1, Integer nb, double objf[], double f[],
    double fjac[], Integer ldfjac, Integer sdfjac, Integer iter[],
    double c[], Integer pdc, double cjac[], Integer ldcjac, Integer sdcjac,
    double clamda[], Integer pdclamda, Integer istate[], Integer pdistate,
    Integer iopts[], double opts[], Nag_Comm *comm, Integer info[],
    NagError *fail)
```

Before calling nag_glopt_nlp_multistart_sqp_lsq (e05usc), the optional parameter arrays **iopts** and **opts** MUST be initialized for use with nag_glopt_nlp_multistart_sqp_lsq (e05usc) by calling nag_glopt_opt_set (e05zkc) with **optstr** set to 'Initialize = e05usc'. Optional parameters may subsequently be specified by calling nag_glopt_opt_set (e05zkc) before the call to nag_glopt_nlp_multistart_sqp_lsq (e05usc).

3 Description

The problem is assumed to be stated in the following form:

$$\underset{x \in R^n}{\text{minimize}} F(x) = \frac{1}{2} \sum_{i=1}^m (y_i - f_i(x))^2 \quad \text{subject to} \quad l \leq \begin{pmatrix} x \\ A_L x \\ c(x) \end{pmatrix} \leq u, \quad (1)$$

where $F(x)$ (the *objective function*) is a nonlinear function which can be represented as the sum of squares of m subfunctions $(y_1 - f_1(x)), (y_2 - f_2(x)), \dots, (y_m - f_m(x))$, the y_i are constant, A_L is an n_L by n constant linear constraint matrix, and $c(x)$ is an n_N element vector of nonlinear constraint functions. (The matrix A_L and the vector $c(x)$ may be empty.) The objective function and the constraint functions are assumed to be smooth, i.e., at least twice-continuously differentiable. (This function will usually solve (1) if any isolated discontinuities are away from the solution.)

nag_glopt_nlp_multistart_sqp_lsq (e05usc) solves a user-specified number of local optimization problems with different starting points. You may specify the starting points via the function **start**. If a random number generator is used to generate the starting points then the argument **repeat1** allows you to specify whether a repeatable set of points are generated or whether different starting points are generated on different calls. The resulting local minima are ordered and the best **nb** results returned in order of ascending values of the resulting objective function values at the minima. Thus the value returned in position 1 will be the best result obtained. If a sufficiently high number of different points are chosen then this is likely to be the global minimum.

4 References

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

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

5 Arguments

- 1: **m** – Integer *Input*
On entry: m , the number of subfunctions associated with $F(x)$.
Constraint: $m > 0$.
- 2: **n** – Integer *Input*
On entry: n , the number of variables.
Constraint: $n > 0$.
- 3: **nclin** – Integer *Input*
On entry: n_L , the number of general linear constraints.
Constraint: $nclin \geq 0$.
- 4: **ncnln** – Integer *Input*
On entry: n_N , the number of nonlinear constraints.
Constraint: $ncnln \geq 0$.
- 5: **a**[*dim*] – const double *Input*
Note: the dimension, *dim*, of the array **a** must be at least $pda \times n$ when $nclin > 0$.
Where $A(i, j)$ appears in this document, it refers to the array element $a[(j - 1) \times pda + i - 1]$.
On entry: the matrix A_L of general linear constraints in (1). That is, $A(i, j)$ must contain the j th coefficient of the i th general linear constraint, for $j = 1, 2, \dots, n$ and $i = 1, 2, \dots, nclin$. If $nclin = 0$ then **a** may be specified as **NULL**.
- 6: **pda** – Integer *Input*
On entry: the stride separating matrix row elements in the array **a**.
Constraint: $pda \geq nclin$.
- 7: **bl**[$n + nclin + ncnln$] – const double *Input*
- 8: **bu**[$n + nclin + ncnln$] – const double *Input*
On entry: **bl** must contain the lower bounds and **bu** the upper bounds for all the constraints in the following order. The first n elements of each array must contain the bounds on the variables, the next n_L elements the bounds for the general linear constraints (if any) and the next n_N elements the bounds for the general nonlinear constraints (if any). To specify a nonexistent lower bound (i.

e., $l_j = -\infty$), set $\mathbf{bl}[j-1] \leq -bigbnd$, and to specify a nonexistent upper bound (i.e., $u_j = +\infty$), set $\mathbf{bu}[j-1] \geq bigbnd$; the default value of $bigbnd$ is 10^{20} , but this may be changed by the optional parameter **Infinite Bound Size**. To specify the j th constraint as an equality, set $\mathbf{bl}[j-1] = \mathbf{bu}[j-1] = \beta$, say, where $|\beta| < bigbnd$.

Constraints:

$\mathbf{bl}[j-1] \leq \mathbf{bu}[j-1]$, for $j = 1, 2, \dots, \mathbf{n} + \mathbf{ncnln} + \mathbf{ncnln}$;
if $\mathbf{bl}[j-1] = \mathbf{bu}[j-1] = \beta$, $|\beta| < bigbnd$.

9: **y[m]** – const double *Input*

On entry: the coefficients of the constant vector y of the objective function.

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

confun must calculate the vector $c(x)$ of nonlinear constraint functions and (optionally) its Jacobian ($= \frac{\partial c}{\partial x}$) for a specified n -element vector x . If there are no nonlinear constraints (i.e., $\mathbf{ncnln} = 0$), **confun** will never be called by `nag_glopt_nlp_multistart_sqp_lsq` (e05usc) and the NAG defined null void function pointer, **NULLFN**, may be supplied in the call instead. If there are nonlinear constraints, the first call to **confun** will occur before the first call to **objfun**.

The specification of **confun** is:

```
void confun (Integer *mode, Integer ncnln, Integer n, Integer pdcjsl,
             const Integer needc[], const double x[], double c[],
             double cjsl[], Integer nstate, Nag_Comm *comm)
```

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

On entry: indicates which values must be assigned during each call of **confun**. Only the following values need be assigned, for each value of i such that $\mathbf{needc}[i-1] > 0$:

mode = 0
 $\mathbf{c}[i-1]$, the i th nonlinear constraint.

mode = 1
All available elements in $\mathbf{CJSL}(i, j)$, for $j = 1, 2, \dots, \mathbf{n}$ (see **cjsl** for the definition of **CJSL**).

mode = 2
 $\mathbf{c}[i-1]$ and all available elements in $\mathbf{CJSL}(i, j)$, for $j = 1, 2, \dots, \mathbf{n}$ (see **cjsl** for the definition of **CJSL**).

On exit: may be set to a negative value if you wish to abandon the solution to the current local minimization problem. In this case `nag_glopt_nlp_multistart_sqp_lsq` (e05usc) will move to the next local minimization problem.

2: **ncnln** – Integer *Input*

On entry: n_N , the number of nonlinear constraints.

3: **n** – Integer *Input*

On entry: n , the number of variables.

4: **pdcjsl** – Integer *Input*

On entry: the stride separating matrix row elements in the array **cjsl**.

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

On entry: the indices of the elements of **c** and/or **cjsl** that must be evaluated by **confun**. If $\mathbf{needc}[i-1] > 0$, $\mathbf{c}[i-1]$ and/or the available elements of $\mathbf{CJSL}(i, j)$, for

$j = 1, 2, \dots, \mathbf{n}$ (see argument **mode**) must be evaluated at x . See **cjsl** for the definition of **CJSL**.

6: **x[n]** – const double *Input*

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

7: **c[ncnln]** – double *Output*

On exit: if **needc**[$i - 1$] > 0 and **mode** = 0 or 2, **c**[$i - 1$] must contain the value of $c_i(x)$. The remaining elements of **c**, corresponding to the non-positive elements of **needc**, need not be set.

8: **cjsl[dim]** – double *Input/Output*

Note: the dimension, dim , of the array **cjsl** is **pdcjsl** \times **n**.

Where **CJSL**(i, j) appears in this document, it refers to the array element **cjsl**[($j - 1$) \times **pdcjsl** + $i - 1$].

CJSL may be regarded as a two-dimensional ‘slice’ in column order of the three-dimensional matrix **CJAC** stored in the array **cjac** of nag_glopt_nlp_multistart_sqplsq (e05usc).

On entry: unless **Derivative Level** = 2 or 3, the elements of **cjsl** are set to special values which enable nag_glopt_nlp_multistart_sqplsq (e05usc) to detect whether they are changed by **confun**.

On exit: if **needc**[$i - 1$] > 0 and **mode** = 1 or 2, **CJSL**(i, j), for $j = 1, 2, \dots, \mathbf{n}$, must contain the available elements of the vector ∇c_i given by

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

where $\frac{\partial c_i}{\partial x_j}$ is the partial derivative of the i th constraint with respect to the j th variable, evaluated at the point x . See also the argument **nstate**. The remaining **CJSL**(i, j), for $j = 1, 2, \dots, \mathbf{n}$, corresponding to non-positive elements of **needc**, need not be set.

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

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

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

- 9: **nstate** – Integer *Input*
On entry: if **nstate** = 1 then nag_glopt_nlp_multistart_sqplsq (e05usc) is calling **confun** for the first time on the current local optimization problem. This argument setting allows you to save computation time if certain data must be read or calculated only once.
- 10: **comm** – Nag_Comm *
 Pointer to structure of type Nag_Comm; the following members are relevant to **confun**.
- user** – double *
iuser – Integer *
p – Pointer
- The type Pointer will be void *. Before calling nag_glopt_nlp_multistart_sqplsq (e05usc) you may allocate memory and initialize these pointers with various quantities for use by **confun** when called from nag_glopt_nlp_multistart_sqplsq (e05usc) (see Section 2.3.1.1 in How to Use the NAG Library and its Documentation).

confun should be tested separately before being used in conjunction with nag_glopt_nlp_multistart_sqplsq (e05usc). See also the description of the optional parameter **Verify**.

- 11: **objfun** – function, supplied by the user *External Function*
objfun must calculate either the i th element of the vector $f(x) = (f_1(x), f_2(x), \dots, f_m(x))^T$ or all m elements of $f(x)$ and (optionally) its Jacobian $(= \frac{\partial f}{\partial x})$ for a specified n -element vector x .

The specification of **objfun** is:

```
void objfun (Integer *mode, Integer m, Integer n, Integer pdfjssl,
             Integer needfi, const double x[], double f[], double fjssl[],
             Integer nstate, Nag_Comm *comm)
```

- 1: **mode** – Integer * *Input/Output*
On entry: indicates which values must be assigned during each call of **objfun**. Only the following values need be assigned:
- mode** = 0 and **needfi** = i , where $i > 0$
 $f[i - 1]$.
- mode** = 0 and **needfi** < 0
 f .
- mode** = 1 and **needfi** < 0
 All available elements of **fjssl**.
- mode** = 2 and **needfi** < 0
 f and all available elements of **fjssl**.
- On exit:* may be set to a negative value if you wish to abandon the solution to the current local minimization problem. In this case nag_glopt_nlp_multistart_sqplsq (e05usc) will move to the next local minimization problem.
- 2: **m** – Integer *Input*
On entry: m , the number of subfunctions.
- 3: **n** – Integer *Input*
On entry: n , the number of variables.

4:	pdfjsl – Integer	<i>Input</i>
	<i>On entry:</i> the stride separating matrix row elements in the array fjsl .	
5:	needfi – Integer	<i>Input</i>
	<i>On entry:</i> if needfi = $i > 0$, only the i th element of $f(x)$ needs to be evaluated at x ; the remaining elements need not be set. This can result in significant computational savings when $m \gg n$.	
6:	x[n] – const double	<i>Input</i>
	<i>On entry:</i> x , the vector of variables at which the objective function and/or all available elements of its gradient are to be evaluated.	
7:	f[m] – double	<i>Output</i>
	<i>On exit:</i> if mode = 0 and needfi = $i > 0$, f [$i - 1$] must contain the value of f_i at x . If mode = 0 or 2 and needfi < 0, f [$i - 1$] must contain the value of f_i at x , for $i = 1, 2, \dots, m$.	
8:	fjsl[dim] – double	<i>Input/Output</i>
	Note: the dimension, dim , of the array fjsl is pdfjsl \times n . The (i, j) th element of the matrix is stored in fjsl [($j - 1$) \times pdfjsl + $i - 1$]. FJSL may be regarded as a two-dimensional ‘slice’ in column order of the three-dimensional matrix FJAC stored in the array fjac of nag_glopt_nlp_multistart_sqplsq (e05usc). <i>On entry:</i> is set to a special value. <i>On exit:</i> if mode = 1 or 2 and needfi < 0, the i th row of fjsl must contain the available elements of the vector ∇f_i given by $\nabla f_i = (\partial f_i / \partial x_1, \partial f_i / \partial x_2, \dots, \partial f_i / \partial x_n)^T,$ evaluated at the point x . See also the argument nstate .	
9:	nstate – Integer	<i>Input</i>
	<i>On entry:</i> if nstate = 1 then nag_glopt_nlp_multistart_sqplsq (e05usc) is calling objfun for the first time on the current local optimization problem. This argument setting allows you to save computation time if certain data must be read or calculated only once.	
10:	comm – Nag_Comm *	
	Pointer to structure of type Nag_Comm; the following members are relevant to objfun . user – double * iuser – Integer * p – Pointer The type Pointer will be void *. Before calling nag_glopt_nlp_multistart_sqplsq (e05usc) you may allocate memory and initialize these pointers with various quantities for use by objfun when called from nag_glopt_nlp_multistart_sqplsq (e05usc) (see Section 2.3.1.1 in How to Use the NAG Library and its Documentation).	

objfun should be tested separately before being used in conjunction with nag_glopt_nlp_multistart_sqplsq (e05usc). See also the description of the optional parameter **Verify**.

- 12: **npts** – Integer *Input*
On entry: the number of different starting points to be generated and used. The more points used, the more likely that the best returned solution will be a global minimum.
Constraint: $1 \leq \mathbf{nb} \leq \mathbf{npts}$.
- 13: **x[*dim*]** – double *Output*
Note: the dimension, *dim*, of the array **x** must be at least $\mathbf{pdx} \times \mathbf{nb}$.
Where **X**(*j*, *i*) appears in this document, it refers to the array element $\mathbf{x}[(i-1) \times \mathbf{pdx} + j - 1]$.
On exit: **X**(*j*, *i*) contains the final estimate of the *i*th solution, for $j = 1, 2, \dots, \mathbf{n}$.
- 14: **pdx** – Integer *Input*
On entry: the first dimension of **X** as stored in the array **x**.
Constraint: $\mathbf{pdx} \geq \mathbf{n}$.
- 15: **start** – function, supplied by the user *External Function*
start must calculate the **npts** starting points to be used by the local optimizer. If you do not wish to write a function specific to your problem then you can specify the NAG defined null void function pointer, NULLFN in the call. In this case, a default function uses the NAG quasi-random number generators to distribute starting points uniformly across the domain. It is affected by the value of **repeat1**.

The specification of **start** is:

```
void start (Integer npts, double quas[], Integer n,
            Nag_Boolean repeat1, const double bl[], const double bu[],
            Nag_Comm *comm, Integer *mode)
```

- 1: **npts** – Integer *Input*
On entry: indicates the number of starting points.
- 2: **quas**[$\mathbf{n} \times \mathbf{npts}$] – double *Input/Output*
Note: where **QUAS**(*j*, *i*) appears in this document, it refers to the array element **quas**[(*i* - 1) × **n** + *j* - 1].
On entry: all elements of **quas** will have been set to zero, so only nonzero values need be set subsequently.
On exit: must contain the starting points for the **npts** local minimizations, i.e., **QUAS**(*j*, *i*) must contain the *j*th component of the *i*th starting point.
- 3: **n** – Integer *Input*
On entry: the number of variables.
- 4: **repeat1** – Nag_Boolean *Input*
On entry: specifies whether a repeatable or non-repeatable sequence of points are to be generated.
- 5: **bl**[**n**] – const double *Input*
On entry: the lower bounds on the variables. These may be used to ensure that the starting points generated in some sense ‘cover’ the region, but there is no requirement that a starting point be feasible.

- | | | |
|----|--|---------------------|
| 6: | bu[n] – const double
<i>On entry:</i> the upper bounds on the variables. (See bl .) | <i>Input</i> |
| 7: | comm – Nag_Comm *
Pointer to structure of type Nag_Comm; the following members are relevant to start .

user – double *
iuser – Integer *
p – Pointer

The type Pointer will be void *. Before calling nag_glopt_nlp_multistart_sqplsq (e05usc) you may allocate memory and initialize these pointers with various quantities for use by start when called from nag_glopt_nlp_multistart_sqplsq (e05usc) (see Section 2.3.1.1 in How to Use the NAG Library and its Documentation). | |
| 8: | mode – Integer *
<i>On entry:</i> mode will contain 0.

<i>On exit:</i> if you set mode to a negative value then nag_glopt_nlp_multistart_sqplsq (e05usc) will terminate immediately with fail.code = NE_USER_STOP. Provided fail is not NAGERR_DEFAULT on entry to nag_glopt_nlp_multistart_sqplsq (e05usc), fail.errnum will contain this value of mode . | <i>Input/Output</i> |
- 16: **repeat1** – Nag_Boolean *Input*
On entry: is passed as an argument to **start** and may be used to initialize a random number generator to a repeatable, or non-repeatable, sequence. See Section 9 for more detail.
- 17: **nb** – Integer *Input*
On entry: the number of solutions to be returned. The function saves up to **nb** local minima ordered by increasing value of the final objective function. If the defining criterion for ‘best solution’ is only that the value of the objective function is as small as possible then **nb** should be set to 1. However, if you want to look at other solutions that may have desirable properties then setting **nb** > 1 will produce **nb** local minima, ordered by increasing value of their objective functions at the minima.
Constraint: $1 \leq \mathbf{nb} \leq \mathbf{npts}$.
- 18: **objf[nb]** – double *Output*
On exit: **objf**[*i* – 1] contains the value of the objective function at the final iterate for the *i*th solution.
- 19: **f[dim]** – double *Output*
Note: the dimension, *dim*, of the array **f** must be at least $\mathbf{m} \times \mathbf{nb}$.
 Where **F**(*j*, *i*) appears in this document, it refers to the array element **f**[(*i* – 1) × **m** + *j* – 1].
On exit: **F**(*j*, *i*) contains the value of the *j*th function *f_j* at the final iterate, for *j* = 1, 2, ..., **m**, for the *i*th solution, for *i* = 1, 2, ..., **nb**.
- 20: **fjac[dim]** – double *Output*
Note: the dimension, *dim*, of the array **fjac** must be at least **ldfjac** × **sdfjac** × **nb**.
 Where **FJAC**(*k*, *j*, *i*) appears in this document, it refers to the array element **fjac**[(*i* – 1) × **ldfjac** × **sdfjac** + (*j* – 1) × **ldfjac** + *k* – 1].

On exit: for the i th returned solution, the Jacobian matrix of the functions f_1, f_2, \dots, f_m at the final iterate, i.e., $\mathbf{FJAC}(k, j, i)$ contains the partial derivative of the k th function with respect to the j th variable, for $k = 1, 2, \dots, \mathbf{m}$, $j = 1, 2, \dots, \mathbf{n}$ and $i = 1, 2, \dots, \mathbf{nb}$. (See also the discussion of argument **fjst** under **objfun**.)

21: **ldfjac** – Integer *Input*

On entry: the first dimension of the matrix **FJAC** as stored in the array **fjac**.

Constraint: **ldfjac** $\geq \mathbf{m}$.

22: **sdfjac** – Integer *Input*

On entry: the second dimension of the matrix **FJAC** as stored in the array **fjac**.

Constraint: **sdfjac** $\geq \mathbf{n}$.

23: **iter[nb]** – Integer *Output*

On exit: **iter**[$i - 1$] contains the number of major iterations performed to obtain the i th solution. If less than **nb** solutions are returned then **iter**[**nb** - 1] contains the number of starting points that have resulted in a converged solution. If this is close to **npts** then this might be indicative that fewer than **nb** local minima exist.

24: **c[dim]** – double *Output*

Note: the dimension, dim , of the array **c** must be at least **pdcc** \times **nb**.

Where **C**(j, i) appears in this document, it refers to the array element **c**[($i - 1$) \times **pdcc** + $j - 1$].

On exit: if **ncnln** > 0 , **C**(j, i) contains the value of the j th nonlinear constraint function c_j at the final iterate, for the i th solution, for $j = 1, 2, \dots, \mathbf{ncnln}$.

If **ncnln** = 0, the array **c** is not referenced and may be specified as **NULL**.

25: **pdcc** – Integer *Input*

On entry: the first dimension of **C** as stored in the array **c**.

Constraint: **pdcc** $\geq \mathbf{ncnln}$.

26: **cjac[dim]** – double *Output*

Note: the dimension, dim , of the array **cjac** must be at least **ldccjac** \times **sdcjac** \times **nb**.

Where **CJAC**(k, j, i) appears in this document, it refers to the array element **cjac**[($i - 1$) \times **ldccjac** \times **sdcjac** + ($j - 1$) \times **ldccjac** + $k - 1$].

On exit: if **ncnln** > 0 , **cjac** contains the Jacobian matrices of the nonlinear constraint functions at the final iterate for each of the returned solutions, i.e., **CJAC**(k, j, i) contains the partial derivative of the k th constraint function with respect to the j th variable, for $k = 1, 2, \dots, \mathbf{ncnln}$ and $j = 1, 2, \dots, \mathbf{n}$, for the i th solution. (See the discussion of argument **cjst** under **confun**.)

If **ncnln** = 0, the array **cjac** is not referenced and may be specified as **NULL**.

27: **ldccjac** – Integer *Input*

On entry: the first dimension of the matrix **CJAC** as stored in the array **cjac**.

Constraint: **ldccjac** $\geq \mathbf{ncnln}$.

28: **sdcjac** – Integer *Input*

On entry: the second dimension of the matrix **CJAC** as stored in the array **cjac**.

Constraint: if **ncnln** > 0 , **sdcjac** $\geq \mathbf{n}$.

29: **clamda**[*dim*] – double *Output*

Note: the dimension, *dim*, of the array **clamda** must be at least **pdclamda** × **nb**.

Where **CLAMDA**(*j*, *i*) appears in this document, it refers to the array element **clamda**[(*i* − 1) × **pdclamda** + *j* − 1].

On exit: the values of the QP multipliers from the last QP subproblem solved for the *i*th solution. **CLAMDA**(*j*, *i*) should be non-negative if **ISTATE**(*j*, *i*) = 1 and non-positive if **ISTATE**(*j*, *i*) = 2.

30: **pdclamda** – Integer *Input*

On entry: the stride separating matrix row elements in the array **clamda**.

Constraint: **pdclamda** ≥ **n** + **nclin** + **ncnln**.

31: **istate**[*dim*] – Integer *Output*

Note: the dimension, *dim*, of the array **istate** must be at least **pdistate** × **nb**.

Where **ISTATE**(*j*, *i*) appears in this document, it refers to the array element **istate**[(*i* − 1) × **pdistate** + *j* − 1].

On exit: **ISTATE**(*j*, *i*) contains the status of the constraints in the QP working set for the *i*th solution. The significance of each possible value of **ISTATE**(*j*, *i*) is as follows:

ISTATE (<i>j</i> , <i>i</i>)	Meaning
0	The constraint is satisfied to within the feasibility tolerance, but is not in the QP working set.
1	This inequality constraint is included in the QP working set at its lower bound.
2	This inequality constraint is included in the QP working set at its upper bound.
3	This constraint is included in the QP working set as an equality. This value of istate can occur only when bl [<i>j</i> − 1] = bu [<i>j</i> − 1].

32: **pdistate** – Integer *Input*

On entry: the stride separating matrix row elements in the array **istate**.

Constraint: **pdistate** ≥ **n** + **nclin** + **ncnln**.

33: **iopts**[740] – Integer *Communication Array*

34: **opts**[485] – double *Communication Array*

The arrays **iopts** and **opts** MUST NOT be altered between calls to any of the functions **nag_glopt_nlp_multistart_sqp_lsq** (e05usc) and **nag_glopt_opt_set** (e05zkc).

35: **comm** – Nag_Comm *

The NAG communication argument (see Section 2.3.1.1 in How to Use the NAG Library and its Documentation).

36: **info**[**nb**] – Integer *Output*

On exit: if **fail.code** = NE_NOERROR, **info**[*i* − 1] contains one of 0, 1 or 6.

info[*i* − 1] = 1

The final iterate *x* satisfies the first-order Kuhn–Tucker conditions (see Section 11 in **nag_opt_nlp_solve** (e04wdc)) to the accuracy requested, but the sequence of iterates has not yet converged. The local optimizer was terminated because no further improvement could be made in the merit function (see Section 9.1).

info[$i - 1$] = 6

x does not satisfy the first-order Kuhn–Tucker conditions (see Section 11) and no improved point for the merit function (see Section 9.1) could be found during the final linesearch.

This sometimes occurs because an overly stringent accuracy has been requested, i.e., the value of the optional parameter **Optimality Tolerance** (default value = $\epsilon_R^{0.8}$, where ϵ_R is the value of the optional parameter **Function Precision** (default value = $\epsilon^{0.9}$, where ϵ is the *machine precision*)) is too small.

As usual 0 denotes success.

If **fail.code** = NW_SOME_SOLUTIONS on exit, then not all **nb** solutions have been found, and **info**[**nb** – 1] contains the number of solutions actually found.

37: **fail** – NagError *

Input/Output

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

6 Error Indicators and Warnings

NE_ALLOC_FAIL

Dynamic memory allocation failed.

See Section 2.3.1.2 in How to Use the NAG Library and its Documentation for further information.

NE_BAD_PARAM

On entry, argument $\langle value \rangle$ had an illegal value.

NE_BOUND

On entry, **bl**[$i - 1$] > **bu**[$i - 1$]: $i = \langle value \rangle$.

Constraint: **bl**[$i - 1$] ≤ **bu**[$i - 1$], for all i .

NE_DERIV_ERRORS

The user-supplied derivatives of the objective function and/or nonlinear constraints appear to be incorrect.

Large errors were found in the derivatives of the objective function and/or nonlinear constraints. This value of **fail.code** will occur if the verification process indicated that at least one gradient or Jacobian element had no correct figures. You should refer to or enable the printed output to determine which elements are suspected to be in error.

As a first-step, you should check that the code for the objective and constraint values is correct – for example, by computing the function at a point where the correct value is known. However, care should be taken that the chosen point fully tests the evaluation of the function. It is remarkable how often the values $x = 0$ or $x = 1$ are used to test function evaluation procedures, and how often the special properties of these numbers make the test meaningless.

Gradient checking will be ineffective if the objective function uses information computed by the constraints, since they are not necessarily computed before each function evaluation.

Errors in programming the function may be quite subtle in that the function value is ‘almost’ correct. For example, the function may not be accurate to full precision because of the inaccurate calculation of a subsidiary quantity, or the limited accuracy of data upon which the function depends. A common error on machines where numerical calculations are usually performed in double precision is to include even one single precision constant in the calculation of the function; since some compilers do not convert such constants to double precision, half the correct figures may be lost by such a seemingly trivial error.

NE_INITIALIZATION

Failed to initialize optional parameter arrays.

NE_INT

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

Constraint: **m** > 0.

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

Constraint: **n** > 0.

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

Constraint: **nclin** ≥ 0.

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

Constraint: **ncnln** ≥ 0.

NE_INT_2

On entry, **ldcjac** = $\langle value \rangle$ and **ncnln** = $\langle value \rangle$.

Constraint: **ldcjac** ≥ **ncnln**.

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

Constraint: **ldfjac** ≥ **m**.

On entry, **nb** = $\langle value \rangle$ and **npts** = $\langle value \rangle$.

Constraint: $1 \leq \mathbf{nb} \leq \mathbf{npts}$.

On entry, **pda** = $\langle value \rangle$ and **nclin** = $\langle value \rangle$.

Constraint: **pda** ≥ **nclin**.

On entry, **pdc** = $\langle value \rangle$ and **ncnln** = $\langle value \rangle$.

Constraint: **pdc** ≥ **ncnln**.

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

Constraint: **pdx** ≥ **n**.

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

Constraint: **sdfjac** ≥ **n**.

NE_INT_3

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

Constraint: if **ncnln** > 0, **sdcjac** ≥ **n**.

NE_INT_4

On entry, **pdclambda** = $\langle value \rangle$, **n** = $\langle value \rangle$, **nclin** = $\langle value \rangle$ and **ncnln** = $\langle value \rangle$.

Constraint: **pdclambda** ≥ **n** + **nclin** + **ncnln**.

On entry, **pdistate** = $\langle value \rangle$, **n** = $\langle value \rangle$, **nclin** = $\langle value \rangle$ and **ncnln** = $\langle value \rangle$.

Constraint: **pdistate** ≥ **n** + **nclin** + **ncnln**.

NE_INTERNAL_ERROR

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

An unexpected error has been triggered by this function. Please contact NAG.

See Section 2.7.6 in How to Use the NAG Library and its Documentation for further information.

NE_LIN_NOT_FEASIBLE

*nag_glopt_nlp_multistart_sqp_lsq (e05usc) has terminated without finding any solutions. The majority of calls to the local optimizer have failed to find a feasible point for the linear constraints and bounds, which means that either no feasible point exists for the given value of the optional parameter **Linear Feasibility Tolerance** (default value $\sqrt{\text{macheps}}$, where *macheps* is*

the **machine precision**), or no feasible point could be found in the number of iterations specified by the optional parameter **Minor Iteration Limit**. You should check that there are no constraint redundancies. If the data for the constraints are accurate only to an absolute precision σ , you should ensure that the value of the optional parameter **Linear Feasibility Tolerance** is greater than σ . For example, if all elements of A_L are of order unity and are accurate to only three decimal places, **Linear Feasibility Tolerance** should be at least 10^{-3} .

NE_NO_LICENCE

Your licence key may have expired or may not have been installed correctly.
See Section 2.7.5 in How to Use the NAG Library and its Documentation for further information.

NE_NO_SOLUTION

nag_glopt_nlp_multistart_sqp_lsq (e05usc) has failed to find any solutions. The majority of local optimizations have failed because the limiting number of iterations have been reached.

NE_NONLIN_NOT_FEASIBLE

nag_glopt_nlp_multistart_sqp_lsq (e05usc) has failed to find any solutions. The majority of local optimizations could not find a feasible point for the nonlinear constraints. The problem may have no feasible solution. This behaviour will occur if there is no feasible point for the nonlinear constraints. (However, there is no general test that can determine whether a feasible point exists for a set of nonlinear constraints.)

NE_USER_STOP

User terminated computation from **start** procedure: **mode** = $\langle value \rangle$.

NW_SOME_SOLUTIONS

Only $\langle value \rangle$ solutions obtained.

Not all **nb** solutions have been found. **info[nb - 1]** contains the number actually found.

7 Accuracy

If **fail.code** = NE_NOERROR on exit and the value of **info**[$i - 1$] = 0, then the vector returned in the array **x** for solution i is an estimate of the solution to an accuracy of approximately **Optimality Tolerance**.

8 Parallelism and Performance

nag_glopt_nlp_multistart_sqp_lsq (e05usc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library. In these implementations, this function may make calls to the user-supplied functions from within an OpenMP parallel region. Thus OpenMP pragmas within the user functions can only be used if you are compiling the user-supplied function and linking the executable in accordance with the instructions in the Users' Note for your implementation. You must also ensure that you use the NAG communication argument **comm** in a thread safe manner, which is best achieved by only using it to supply read-only data to the user functions.

nag_glopt_nlp_multistart_sqp_lsq (e05usc) makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the x06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this function. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 Further Comments

You should be wary of requesting much intermediate output from the local optimizer, since large volumes may be produced if **npts** is large.

In computing the default set of starting points, `nag_glopt_nlp_multistart_sqp_lsq` (e05usc) makes use of the NAG quasi-random Sobol generator (`nag_quasi_init` (g05ylc) and `nag_quasi_rand_uniform` (g05ymc)). If `NULLFN` is used as the actual argument for **start** and **repeat1** = `Nag.FALSE` then a randomly chosen value for **iskip** is used, otherwise **iskip** is set to 100. If **repeat1** is set to `Nag.FALSE` and the program is executed several times, each time producing the same best answer, then there is increased probability that this answer is a global minimum. However, if it is important that identical results be obtained on successive runs, then **repeat1** should be set to `Nag.TRUE`.

9.1 Description of the Printed Output

This section describes the intermediate printout and final printout that may be produced by `nag_glopt_nlp_multistart_sqp_lsq` (e05usc). The intermediate printout is a subset of the monitoring information produced by the function at every iteration (see Section 13). You can control the level of printed output (see the description of the optional parameters **Major Print Level** and **Minor Print Level**). Note that the intermediate printout and final printout are produced only if **Major Print Level** ≥ 10 or **Minor Print Level** ≥ 10 .

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

Maj	is the major iteration count.
Mnr	is the number of minor iterations required by the feasibility and optimality phases of the QP subproblem. Generally, Mnr will be 1 in the later iterations, since theoretical analysis predicts that the correct active set will be identified near the solution (see Section 11). 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 α_k taken along the computed search direction. On reasonably well-behaved local problems, the unit step (i.e., $\alpha_k = 1$) will be taken as the solution is approached.
Merit Function	is the value of the augmented Lagrangian merit function (12) in <code>nag_opt_nlp_revcomm</code> (e04ufc) at the current iterate. This function will decrease at each iteration unless it was necessary to increase the penalty parameters (see Section 11 in <code>nag_opt_nlp_solve</code> (e04wdc)). As the solution is approached, Merit Function will converge to the value of the objective function at the solution. If the QP subproblem does not have a feasible point (signified by I at the end of the current output line) then the merit function is a large multiple of the constraint violations, weighted by the penalty parameters. During a sequence of major iterations with infeasible subproblems, the sequence of Merit Function values will decrease monotonically until either a feasible subproblem is obtained or the local optimizer terminates. Repeated failures will prevent a feasible point being found for the nonlinear constraints. If there are no nonlinear constraints present (i.e., ncnln = 0) then this entry contains Objective , the value of the objective function $F(x)$. The objective function will decrease monotonically to its optimal value when there are no nonlinear constraints.
Norm Gz	is $\ Z^T g_{FR}\ $, the Euclidean norm of the projected gradient (see Section 11 in <code>nag_opt_nlp_solve</code> (e04wdc)). Norm Gz will be approximately zero in the neighbourhood of a solution.

Violtn	is the Euclidean norm of the residuals of constraints that are violated or in the predicted active set (not printed if ncnln is zero). Violtn will be approximately zero in the neighbourhood of a solution.
Cond Hz	is a lower bound on the condition number of the projected Hessian approximation H_Z ($H_Z = Z^T H_{FR} Z = R_Z^T R_Z$; see (6) and (11) in nag_opt_nlp_revcomm (e04ufc)). The larger this number, the more difficult the local problem.
M	is printed if the quasi-Newton update has been modified to ensure that the Hessian approximation is positive definite (see Section 11 in nag_opt_nlp_solve (e04wdc)).
I	is printed if the QP subproblem has no feasible point.
C	is printed if central differences have been used to compute the unspecified objective and constraint gradients. If the value of Step is zero then the switch to central differences was made because no lower point could be found in the linesearch. (In this case, the QP subproblem is resolved with the central difference gradient and Jacobian.) If the value of Step is nonzero then central differences were computed because Norm Gz and Violtn imply that x is close to a Kuhn–Tucker point (see Section 11 in nag_opt_nlp_solve (e04wdc)).
L	is printed if the linesearch has produced a relative change in x greater than the value defined by the optional parameter Step Limit . If this output occurs frequently during later iterations of the run, optional parameter Step Limit should be set to a larger value.
R	is printed if the approximate Hessian has been refactorized. If the diagonal condition estimator of R indicates that the approximate Hessian is badly conditioned then the approximate Hessian is refactorized using column interchanges. If necessary, R is modified so that its diagonal condition estimator is bounded.

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.

Itn	is the iteration count.
Step	is the step taken along the computed search direction. If a constraint is added during the current iteration (i.e., Jadd is positive), Step will be the step to the nearest constraint. During the optimality phase, the step can be greater than one only if the factor R_Z is singular. (See Section 11.)
Ninf	is the number of violated constraints (infeasibilities). This will be zero during the optimality phase.
Sinf/Objective	is the value of the current objective function. If x is not feasible, Sinf gives a weighted sum of the magnitudes of constraint violations. If x is feasible, Objective is the value of the objective function of the QP subproblem. The output line for the final iteration of the feasibility phase (i.e., the first iteration for which Ninf is zero) will give the value of the true objective at the first feasible point. During the optimality phase the value of the objective function will be nonincreasing. During the feasibility phase the number of constraint infeasibilities will not increase until either a feasible point is found or the optimality of the multipliers implies that no feasible point exists. Once optimal multipliers are obtained the number of infeasibilities can increase, but the sum of infeasibilities will either remain constant or be reduced until the minimum sum of infeasibilities is found.
Norm Gz	is $\ Z_1^T g_{FR}\ $, the Euclidean norm of the reduced gradient with respect to Z_1 . During the optimality phase, this norm will be approximately zero after a unit step. (See Section 11.)

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.

Varbl	gives the name (v) and index j , for $j = 1, 2, \dots, n$, of the variable.
State	gives the state of the variable (FR if neither bound is in the working set, EQ if a fixed variable, LL if on its lower bound, UL if on its upper bound, TF if temporarily fixed at its current value). If Value lies outside the upper or lower bounds by more than the Feasibility Tolerance , State will be ++ or -- respectively. (The latter situation can occur only when there is no feasible point for the bounds and linear constraints.) A key is sometimes printed before State. A <i>Alternative optimum possible</i> . The variable is active at one of its bounds, but its Lagrange multiplier is essentially zero. This means that if the variable were allowed to start moving away from its bound then there would be no change to the objective function. The values of the other free variables <i>might</i> change, giving a genuine alternative solution. However, if there are any degenerate variables (labelled D), the actual change might prove to be zero, since one of them could encounter a bound immediately. In either case the values of the Lagrange multipliers might also change. D <i>Degenerate</i> . The variable is free, but it is equal to (or very close to) one of its bounds. I <i>Infeasible</i> . The variable is currently violating one of its bounds by more than the Feasibility Tolerance .
Value	is the value of the variable at the final iteration.
Lower Bound	is the lower bound specified for the variable. None indicates that $\mathbf{bl}[j-1] \leq -bigbnd$.
Upper Bound	is the upper bound specified for the variable. None indicates that $\mathbf{bu}[j-1] \geq bigbnd$.
Lagr Mult	is the Lagrange multiplier for the associated bound. This will be zero if State is FR unless $\mathbf{bl}[j-1] \leq -bigbnd$ and $\mathbf{bu}[j-1] \geq bigbnd$, in which case the entry will be blank. If x is optimal, the multiplier should be non-negative if State is LL and non-positive if State is UL.
Slack	is the difference between the variable Value and the nearer of its (finite) bounds $\mathbf{bl}[j-1]$ and $\mathbf{bu}[j-1]$. A blank entry indicates that the associated variable is not bounded (i.e., $\mathbf{bl}[j-1] \leq -bigbnd$ and $\mathbf{bu}[j-1] \geq bigbnd$).

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

L Con	gives the name (L) and index j , for $j = 1, 2, \dots, n_L$, of the linear constraint.
N Con	gives the name (N) and index $(j - n_L)$, for $j = n_L + 1, \dots, n_L + n_N$, of the nonlinear constraint.

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

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

10 Example

This example is based on Problem 57 in Hock and Schittkowski (1981) and involves the minimization of the sum of squares function

$$F(x) = \frac{1}{2} \sum_{i=1}^{44} (y_i - f_i(x))^2,$$

where

$$f_i(x) = x_1 + (0.49 - x_1)e^{-x_2(a_i-8)}$$

and

i	y_i	a_i	i	y_i	a_i
1	0.49	8	23	0.41	22
2	0.49	8	24	0.40	22
3	0.48	10	25	0.42	24
4	0.47	10	26	0.40	24
5	0.48	10	27	0.40	24
6	0.47	10	28	0.41	26
7	0.46	12	29	0.40	26
8	0.46	12	30	0.41	26
9	0.45	12	31	0.41	28
10	0.43	12	32	0.40	28
11	0.45	14	33	0.40	30
12	0.43	14	34	0.40	30
13	0.43	14	35	0.38	30
14	0.44	16	36	0.41	32
15	0.43	16	37	0.40	32
16	0.43	16	38	0.40	34
17	0.46	18	39	0.41	36
18	0.45	18	40	0.38	36
19	0.42	20	41	0.40	38
20	0.42	20	42	0.40	38
21	0.43	20	43	0.39	40
22	0.41	22	44	0.39	42

subject to the bounds

$$\begin{aligned} x_1 &\geq 0.4 \\ x_2 &\geq -4.0 \end{aligned}$$

to the general linear constraint

$$x_1 + x_2 \geq 1.0$$

and to the nonlinear constraint

$$0.49x_2 - x_1x_2 \geq 0.09.$$

The optimal solution (to five figures) is

$$x^* = (0.41995, 1.28484)^T,$$

and $F(x^*) = 0.01423$. The nonlinear constraint is active at the solution.

10.1 Program Text

```
/* nag_glopt_nlp_multistart_sqp_ls (e05usc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

#include <stdio.h>
#include <math.h>
#include <nag.h>
#include <nag_stdlib.h>
```

```

#include <nage05.h>
#include <nagf16.h>
#include <nagg05.h>

#ifdef __cplusplus
extern "C"
{
#endif
    static void NAG_CALL confun(Integer *mode, Integer ncnln, Integer n,
                                Integer pdcj, const Integer needc[],
                                const double x[], double c[], double cjac[],
                                Integer nstate, Nag_Comm *comm);
    static void NAG_CALL objfun(Integer *mode, Integer m, Integer n,
                                Integer pdfj, Integer needfi, const double x[],
                                double f[], double fjac[], Integer nstate,
                                Nag_Comm *comm);
    static void NAG_CALL mystart(Integer npts, double quas[], Integer n,
                                Nag_Boolean repeat, const double bl[],
                                const double bu[], Nag_Comm *comm,
                                Integer *mode);
#ifdef __cplusplus
}
#endif

int main(void)
{
#define LEN_OPTS 485
#define LEN_IOPTS 740

#define ISTATE(I,J) istate[(J-1)* pdistate + I-1]
#define A(I,J) a[(J-1)* pda + I-1]
#define C(I,J) c[(J-1)* pdc + I-1]
#define CLAMDA(I,J) clamda[(J-1)* pdclamda + I-1]
#define X(I,J) x[(J-1)* pdx + I-1]

    static double ruser[3] = { -1.0, -1.0, -1.0 };
    Integer exit_status = 0;
    Integer m = 44, n = 2, nb = 1, nclin = 1, ncnln = 1, npts = 3;
    Integer pdistate, pda, pdc, ldcjac, pdclamda, ldfjac, pdx;
    Integer sdcjac, sdfjac;
    Integer i, j, k, l;
    Nag_Boolean repeat = Nag_TRUE;
    Integer inc;
    double alpha, beta;
    double *a = 0, *bl = 0, *bu = 0, *c = 0, *cjac = 0, *clamda = 0, *f = 0;
    double *fjac = 0, *objf = 0, *work = 0, *x = 0, *y = 0;
    Integer *info = 0, *istate = 0, *iter = 0;
    double opts[LEN_OPTS];
    Integer iopts[LEN_IOPTS];
    Integer len_opts = LEN_OPTS, len_iopts = LEN_IOPTS;
    /* Nag Types */
    Nag_Comm comm;
    NagError fail;

    INIT_FAIL(fail);

    printf("nag_glopt_nlp_multistart_sqp_lsq (e05usc) Example Program Results\n");

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

    fflush(stdout);

    pda = nclin;
    pdc = ncnln;
    ldcjac = ncnln;
    sdcjac = (ncnln > 0 ? n : 0);
    ldfjac = m;
    sdfjac = n;
    pdclamda = n + nclin + ncnln;
    pdistate = n + nclin + ncnln;

```

```

pdx = n;

if (nclin > 0) {
    if (!(a = NAG_ALLOC(pda * n, double)))
    {
        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }
}

if (!(bl = NAG_ALLOC(n + nclin + ncnln, double)) ||
    !(bu = NAG_ALLOC(n + nclin + ncnln, double)) ||
    !(y = NAG_ALLOC(m, double)) ||
    !(c = NAG_ALLOC(pdc * nb, double)) ||
    !(cjac = NAG_ALLOC(ldcjac * sdcjac * nb, double)) ||
    !(f = NAG_ALLOC(m * nb, double)) ||
    !(fjac = NAG_ALLOC(ldfjac * sdfjac * nb, double)) ||
    !(clamda = NAG_ALLOC(pdclamda * nb, double)) ||
    !(x = NAG_ALLOC(pdx * nb, double)) ||
    !(objf = NAG_ALLOC(nb, double)) ||
    !(istate = NAG_ALLOC(pdystate * nb, Integer)) ||
    !(info = NAG_ALLOC(nb, Integer)) ||
    !(iter = NAG_ALLOC(nb, Integer)) || !(work = NAG_ALLOC(nclin, double)))
{
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
}

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

    if (nclin > 0) {
        for (i = 1; i <= nclin; i++)
            for (j = 1; j <= n; j++)
#ifdef _WIN32
                scanf_s("%lf", &A(i, j));
#else
                scanf("%lf", &A(i, j));
#endif
    }
#ifdef _WIN32
    scanf_s("%*[\n] ");
#else
    scanf("%*[\n] ");
#endif
}

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

    for (i = 0; i < (n + nclin + ncnln); i++)
#ifdef _WIN32
        scanf_s("%lf", &bl[i]);
#else
        scanf("%lf", &bl[i]);
#endif
#ifdef _WIN32

```

```

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

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

/* nag_glopt_opt_set (e05zkc).
 * Option setting routine for nag_glopt_nlp_multistart_sqp_lsq (e05usc).
 * First initialize.
 */
nag_glopt_opt_set("Initialize = e05usc",
                  iopts, len_iopts, opts, len_opts, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_glopt_opt_set (e05zkc).\\n%s\\n", fail.message);
    exit_status = 1;
    goto END;
}

/* nag_glopt_nlp_multistart_sqp_lsq (e05usc).
 * Global optimization of a sum of squares problem using multi-start,
 * nonlinear constraints.
 * Solve the problem.
 */
nag_glopt_nlp_multistart_sqp_lsq(m, n, nclin, ncnln, a, pda, bl, bu, y,
                                confun, objfun, npts, x, pdx, mystart,
                                repeat, nb, objf, f, fjac, ldfjac, sdfjac,
                                iter, c, pdc, cjac, ldcjac, sdcjac,
                                clamda, pdclamda, istate, pdistate,
                                iopts, opts, &comm, info, &fail);

if (fail.code != NE_NOERROR && fail.code != NW_SOME_SOLUTIONS) {
    printf("Error from nag_glopt_nlp_multistart_sqp_lsq (e05usc).\\n%s\\n",
          fail.message);
    exit_status = 4;
    goto END;
}

switch (fail.code) {
case NE_NOERROR:
    l = nb;
    break;
case NW_SOME_SOLUTIONS:
    l = info[nb - 1];
    printf("%16" NAG_IFMT " starting points converged\\n", iter[nb - 1]);
    break;
}

for (i = 1; i <= l; i++) {
    printf("\\nSolution number %16" NAG_IFMT "\\n", i);
    printf("\\nLocal minimization exited with code %" NAG_IFMT "\\n",
          info[i - 1]);
    printf("\\nVarbl   Istate   Value           Lagr Mult\\n\\n");
    for (j = 1; j <= n; j++) {
        printf("V %3" NAG_IFMT " %3" NAG_IFMT, j, ISTATE(j, i));
        printf(" %14.6f %12.4f\\n", X(j, i), CLAMDA(j, i));
    }
    if (nclin > 0) {
        /* Below is a call to the NAG version of the level 2 BLAS
         * routine nag_dgemv.
         * This performs the matrix vector multiplication A*X

```

```

    * (linear constraint values) and puts the result in
    * the first nclin locations of work.
    */
    inc = 1;
    alpha = 1.0;
    beta = 0.0;

    /* nag_dgemv (f16pac).
    * Matrix-vector product, real rectangular matrix.
    */
    nag_dgemv(Nag_ColMajor, Nag_NoTrans, nclin, n, alpha, a, pda, &X(1, i),
              inc, beta, work, inc, &fail);
    if (fail.code != NE_NOERROR) {
        printf("Error from nag_dgemv (f16pac).\n%s\n", fail.message);
        exit_status = 5;
        goto END;
    }

    printf("\nL Con  Istate  Value          Lagr Mult\n\n");
    for (k = n + 1; k <= n + nclin; k++) {
        j = k - n;
        printf("L %3" NAG_IFMT " %3" NAG_IFMT, j, ISTATE(k, i));
        printf(" %14.6f %12.4f\n", work[j - 1], CLAMDA(k, i));
    }
    if (ncnln > 0) {
        printf("\nN Con  Istate  Value          Lagr Mult\n\n");
        for (k = n + nclin + 1; k <= n + nclin + ncnln; k++) {
            j = k - n - nclin;
            printf("N %3" NAG_IFMT " %3" NAG_IFMT, j, ISTATE(k, i));
            printf(" %14.6f %12.4f\n", C(j, i), CLAMDA(k, i));
        }
    }
    printf("\nFinal objective value = %15.7f\n", objf[i - 1]);
    printf("\nQP multipliers\n");
    for (k = 1; k <= n + nclin + ncnln; k++)
        printf("%12.4f\n", CLAMDA(k, i));

    if (l == 1)
        break;

    printf("\n-----\n");
}

END:
    NAG_FREE(a);
    NAG_FREE(b1);
    NAG_FREE(bu);
    NAG_FREE(c);
    NAG_FREE(cjac);
    NAG_FREE(clamda);
    NAG_FREE(f);
    NAG_FREE(fjac);
    NAG_FREE(x);
    NAG_FREE(y);
    NAG_FREE(work);
    NAG_FREE(objf);
    NAG_FREE(istate);
    NAG_FREE(info);
    NAG_FREE(iter);
    return exit_status;
}

static void NAG_CALL confun(Integer *mode, Integer ncnln, Integer n,
                           Integer pdcj, const Integer needc[],
                           const double x[], double c[], double cjac[],
                           Integer nstate, Nag_Comm *comm)
{
#define CJAC(I, J) cjac[(J-1) * pdcj + I-1]
    /* Function to evaluate the nonlinear constraint and its 1st derivatives. */
    Integer i, j;

```

```

#pragma omp master
if (comm->user[0] == -1.0) {
    fflush(stdout);
    printf("(User-supplied callback confun, first invocation.)\n");
    comm->user[0] = 0.0;
    fflush(stdout);
}

/* This problem has only one constraint.
 * As an example of using the mode mechanism,
 * terminate if any other size is supplied.
 */
if (ncnln != 1) {
    *mode = -1;
    return;
}

if (nstate == 1) {
    /* First call to confun. Set all Jacobian elements to zero.
     * Note that this will only work when 'Derivative Level = 3'
     * (the default; see Section 11.1).
     */
    for (i = 1; i <= ncnln; i++)
        for (j = 1; j <= n; j++)
            CJAC(i, j) = 0.0;
}

if (needc[0] > 0) {
    if (*mode == 0 || *mode == 2)
        c[0] = -0.09 - x[0] * x[1] + 0.49 * x[1];

    if (*mode == 1 || *mode == 2) {
        CJAC(1, 1) = -x[1];
        CJAC(1, 2) = -x[0] + 0.49;
    }
}
}

static void NAG_CALL objfun(Integer *mode, Integer m, Integer n, Integer pdfj,
                             Integer needfi, const double x[], double f[],
                             double fjac[], Integer nstate, Nag_Comm *comm)
{
#define FJAC(I, J) fjac[J * pdfj + I]

    /* Function to evaluate the subfunctions and their 1st derivatives. */
    double a[] = { 8.0, 8.0, 10.0, 10.0, 10.0, 10.0, 12.0, 12.0, 12.0,
                   12.0, 14.0, 14.0, 14.0, 16.0, 16.0, 16.0, 18.0, 18.0,
                   20.0, 20.0, 20.0, 22.0, 22.0, 22.0, 24.0, 24.0, 24.0,
                   26.0, 26.0, 26.0, 28.0, 28.0, 30.0, 30.0, 30.0, 32.0,
                   32.0, 34.0, 36.0, 36.0, 38.0, 38.0, 40.0, 42.0 };
    double temp, x1, x2;
    Integer i;

#pragma omp master
if (comm->user[1] == -1.0) {
    fflush(stdout);
    printf("(User-supplied callback objfun, first invocation.)\n");
    comm->user[1] = 0.0;
    fflush(stdout);
}

/* This is a two-dimensional objective function.
 * As an example of using the mode mechanism,
 * terminate if any other problem size is supplied.
 */
if (n != 2) {
    *mode = -1;
    return;
}

```

```

    if (nstate == 1) {
        /* This is the first call.
         * Take any special action here if desired.
         */
    }

    x1 = x[0];
    x2 = x[1];

    if (*mode == 0 && needfi > 0) {
        f[needfi - 1] = x1 + (0.49 - x1) * exp(-x2 * (a[needfi - 1] - 8.0));
        return;
    }

    for (i = 0; i < m; i++) {
        temp = exp(-x2 * (a[i] - 8.0));

        if (*mode == 0 || *mode == 2)
            f[i] = x1 + (0.49 - x1) * temp;

        if (*mode == 1 || *mode == 2) {
            FJAC(i, 0) = 1.0 - temp;
            FJAC(i, 1) = -(0.49 - x1) * (a[i] - 8.0) * temp;
        }
    }

    return;
}

static void NAG_CALL mystart(Integer npts, double quas[], Integer n,
                             Nag_Boolean repeat, const double bl[],
                             const double bu[], Nag_Comm *comm, Integer *mode)
{
#define QUAS(I,J) quas[(J-1) * n + I-1]

    if (comm->user[2] == -1.0) {
        fflush(stdout);
        printf("(User-supplied callback mystart, first invocation.)\n");
        comm->user[2] = 0.0;
        fflush(stdout);
    }

    /* All elements of quas[n*npts] are pre-assigned to zero,
     * so we only need to set nonzero elements.
     */
    if (repeat == Nag_TRUE) {
        QUAS(1, 1) = 0.4;
        QUAS(2, 2) = 1.0;
    }
    else {
        /* Generate a non-repeatable spread of points between bl and bu. */
        Nag_BaseRNG genid;
        Integer i, j, lstate, subid;
        Integer *state = 0;
        NagError fail;

        INIT_FAIL(fail);

        genid = Nag_WichmannHill_I;
        subid = 53;
        lstate = -1;

        nag_rand_init_nonrepeatable(genid, subid, NULL, &lstate, &fail);
        if (fail.code != NE_NOERROR) {
            *mode = -1;
            return;
        }

        if (!(state = NAG_ALLOC(lstate, Integer)))
            {

```

```

        *mode = -1;
        return;
    }

    nag_rand_init_nonrepeatable(genid, subid, state, &lstate, &fail);
    if (fail.code != NE_NOERROR) {
        *mode = -1;
        goto END;
    }

    for (j = 2; j <= npts; j++)
        for (i = 1; i <= n; i++) {
            nag_rand_uniform(1, bl[i - 1], bu[i - 1], state, &QUAS(i, j), &fail);
            if (fail.code != NE_NOERROR) {
                *mode = -1;
                goto END;
            }
        }

    END:
    NAG_FREE(state);
}

#undef QUAS
}

```

10.2 Program Data

```

nag_glopt_nlp_multistart_sqp_lsq (e05usc) Example Program Data
 1.0   1.0                                     : matrix a
 0.49  0.49  0.48  0.47  0.48  0.47  0.46  0.46  0.45  0.43  0.45
 0.43  0.43  0.44  0.43  0.43  0.46  0.45  0.42  0.42  0.43  0.41
 0.41  0.40  0.42  0.40  0.40  0.41  0.40  0.41  0.41  0.40  0.40
 0.40  0.38  0.41  0.40  0.40  0.41  0.38  0.40  0.40  0.39  0.39 : y
 0.4      -4.0      1.0      0.0                                     : bl
 1.0e+25  1.0e+25  1.0e+25  1.0e+25                                     : bu
 0.4      0.0                                                         : x

```

10.3 Program Results

```

nag_glopt_nlp_multistart_sqp_lsq (e05usc) Example Program Results
(User-supplied callback mystart, first invocation.)
(User-supplied callback confun, first invocation.)
(User-supplied callback objfun, first invocation.)

```

Solution number 1

Local minimization exited with code 0

Varbl	Istate	Value	Lagr	Mult
V 1	0	0.419953	0.0000	
V 2	0	1.284845	0.0000	

L Con	Istate	Value	Lagr	Mult
L 1	0	1.704798	0.0000	

N Con	Istate	Value	Lagr	Mult
N 1	1	-0.000000	0.0334	

Final objective value = 0.0142298

QP multipliers

0.0000
0.0000
0.0000
0.0334

11 Algorithmic Details

nag_glopt_nlp_multistart_sqp_lsq (e05usc) implements a sequential quadratic programming (SQP) method incorporating an augmented Lagrangian merit function and a BFGS (Broyden–Fletcher–Goldfarb–Shanno) quasi-Newton approximation to the Hessian of the Lagrangian, and is based on nag_opt_nlp_solve (e04wdc). The documents for nag_opt_nlp_revcomm (e04ufc) and nag_opt_nlp_solve (e04wdc) should be consulted for details of the method.

12 Optional Parameters

Several optional parameters in nag_glopt_nlp_multistart_sqp_lsq (e05usc) define choices in the problem specification or the algorithm logic. In order to reduce the number of formal arguments of nag_glopt_nlp_multistart_sqp_lsq (e05usc) 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. The following is a list of the optional parameters available and a full description of each optional parameter is provided in Section 12.1.

Central Difference Interval

Crash Tolerance

Defaults

Derivative Level

Difference Interval

Feasibility Tolerance

Function Precision

Infinite Bound Size

Infinite Step Size

Iteration Limit

Iters

Itns

Linear Feasibility Tolerance

Line Search Tolerance

List

Major Iteration Limit

Major Print Level

Minor Iteration Limit

Minor Print Level

Monitoring File

Nolist

Nonlinear Feasibility Tolerance

Optimality Tolerance

Out_Level

Print Level

Punch Unit

Start Constraint Check At Variable

Start Objective Check At Variable

Step Limit

Stop Constraint Check At Variable

Stop Objective Check At Variable

Verify

Verify Constraint Gradients**Verify Gradients****Verify Level****Verify Objective Gradients**

Optional parameters may be specified by calling `nag_glopt_opt_set` (e05zkc) before a call to `nag_glopt_nlp_multistart_sqp_lsq` (e05usc). Before calling `nag_glopt_nlp_multistart_sqp_lsq` (e05usc), the optional parameter arrays **iopts** and **opts** MUST be initialized for use with `nag_glopt_nlp_multistart_sqp_lsq` (e05usc) by calling `nag_glopt_opt_set` (e05zkc) with **optstr** set to 'Initialize = e05usc'.

All optional parameters not specified are set to their default values. Optional parameters specified are unaltered by `nag_glopt_nlp_multistart_sqp_lsq` (e05usc) (unless they define invalid values) and so remain in effect for subsequent calls to `nag_glopt_nlp_multistart_sqp_lsq` (e05usc).

12.1 Description of the Optional Parameters

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

The summary line contains:

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

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

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

Keywords and character values are case insensitive, however they must be separated by at least one whitespace.

Optional parameters used to specify files have type `Nag_FileID` (see Section 2.3.1.1 in How to Use the NAG Library and its Documentation). This ID value must either be set to 0 (the default value) in which case there will be no output, or will be as returned by a call of `nag_open_file` (x04acc).

For `nag_glopt_nlp_multistart_sqp_lsq` (e05usc) the maximum length of the argument **cvalue** used by `nag_glopt_opt_get` (e05zlc) is 11.

Central Difference Interval *r* Default values are computed

If the algorithm switches to central differences because the forward-difference approximation is not sufficiently accurate, the value of *r* is used as the difference interval for every element of *x*. 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 9.1). The use of finite differences is discussed further under the optional parameter **Difference Interval**.

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

Crash Tolerance *r* Default = 0.01

This value is used when the local minimizer selects an initial working set. If $0 \leq r \leq 1$, the initial working set will include (if possible) bounds or general inequality constraints that lie within *r* of their bounds. In particular, a constraint of the form $a_j^T x \geq l$ will be included in the initial working set if $|a_j^T x - l| \leq r(1 + |l|)$. If $r < 0$ or $r > 1$, the default value is used.

Defaults

This special keyword is used to reset all optional parameters to their default values, and any random state stored in **state** will be destroyed.

Any option value given with this keyword will be ignored. This optional parameter cannot be queried or got.

Derivative Level i Default = 3

This parameter indicates which derivatives are provided in user-supplied functions **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 elements of the objective gradient are not specified.
1	All elements of the objective gradient are provided, but some elements of the constraint Jacobian are not specified.
0	Some elements of both the objective gradient and the constraint Jacobian are not specified.

The value $i = 3$ should be used whenever possible, since `nag_glopt_nlp_multistart_sqp_lsq` (e05usc) is more reliable (and will usually be more efficient) when all derivatives are exact.

If $i = 0$ or 2, `nag_glopt_nlp_multistart_sqp_lsq` (e05usc) will estimate the unspecified elements of the objective gradient, using finite differences. The computation of finite difference approximations usually increases the total run-time, since a call to **objfun** is required for each unspecified element. Furthermore, less accuracy can be attained in the solution (see Chapter 8 of Gill *et al.* (1981), for a discussion of limiting accuracy).

If $i = 0$ or 1, `nag_glopt_nlp_multistart_sqp_lsq` (e05usc) will approximate unspecified elements of the constraint Jacobian. One call to **confun** is needed for each variable for which partial derivatives are not available. For example, if the Jacobian has the form

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

where ‘*’ indicates an element provided by you and ‘?’ indicates an unspecified element, the local minimizer 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 **objfun** and **confun** are needed. (The switch to central differences is not under your control.)

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

Difference Interval r Default values are computed

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

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

In general, a derivative with respect to the j th variable is approximated using the interval δ_j , where $\delta_j = r(1 + |\hat{x}_j|)$, with \hat{x} the first point feasible with respect to the bounds and linear constraints. If the functions are well scaled, the resulting derivative approximation should be accurate to $O(r)$. See Gill *et al.* (1981) for a discussion of the accuracy in finite difference approximations.

If a difference interval is not specified, a finite difference interval will be computed automatically for each variable by a procedure that requires up to six calls of **confun** and **objfun** for each element. This option is recommended if the function is badly scaled or you wish to have the local minimizer

determine constant elements in the objective and constraint gradients (see the descriptions of **confun** and **objfun** in Section 5).

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

Feasibility Tolerance

 r Default = $\sqrt{\epsilon}$

The scalar r defines the maximum acceptable *absolute* violations in linear and nonlinear constraints at a ‘feasible’ point; i.e., a constraint is considered satisfied if its violation does not exceed r . If $r < \epsilon$ or $r \geq 1$, the default value is used. Using this keyword sets both optional parameters **Linear Feasibility Tolerance** and **Nonlinear Feasibility Tolerance** to r , if $\epsilon \leq r < 1$. (Additional details are given under the descriptions of these optional parameters.)

Function Precision

 r Default = $\epsilon^{0.9}$

This parameter defines ϵ_r , which is intended to be a measure of the accuracy with which the problem functions $F(x)$ and $c(x)$ can be computed. If $r < \epsilon$ or $r \geq 1$, the default value is used.

The value of ϵ_r should reflect the relative precision of $1 + |F(x)|$; i.e., ϵ_r acts as a relative precision when $|F|$ is large, and as an absolute precision when $|F|$ is small. For example, if $F(x)$ is typically of order 1000 and the first six significant digits are known to be correct, an appropriate value for ϵ_r would be 10^{-6} . In contrast, if $F(x)$ is typically of order 10^{-4} and the first six significant digits are known to be correct, an appropriate value for ϵ_r would be 10^{-10} . The choice of ϵ_r can be quite complicated for badly scaled problems; see Chapter 8 of Gill *et al.* (1981) for a discussion of scaling techniques. The default value is appropriate for most simple functions that are computed with full accuracy. However, when the accuracy of the computed function values is known to be significantly worse than full precision, the value of ϵ_r should be large enough so that nag_glopt_nlp_multistart_sqp_lsq (e05usc) will not attempt to distinguish between function values that differ by less than the error inherent in the calculation.

Infinite Bound Size

 r Default = 10^{20}

This defines the ‘infinite’ bound *infbnd* in the definition of the problem constraints. Any upper bound greater than or equal to *infbnd* will be regarded as ∞ (and similarly any lower bound less than or equal to $-infbnd$ will be regarded as $-\infty$).

Constraint: $r_{\max}^{\frac{1}{4}} \leq infbnd \leq r_{\max}^{\frac{1}{2}}$.

Infinite Step Size

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

If $r > 0$, r specifies the magnitude of the change in variables that is treated as a step to an unbounded solution. If the change in x during an iteration would exceed the value of r , the objective function is considered to be unbounded below in the feasible region. If $r \leq 0$, the default value is used.

Line Search Tolerance

 r

Default = 0.9

The value r ($0 \leq r < 1$) controls the accuracy with which the step α taken during each iteration approximates a minimum of the merit function along the search direction (the smaller the value of r , the more accurate the linesearch). The default value $r = 0.9$ requests an inaccurate search, and is appropriate for most problems, particularly those with any nonlinear constraints.

If there are no nonlinear constraints, a more accurate search may be appropriate when it is desirable to reduce the number of major iterations – for example, if the objective function is cheap to evaluate, or if a substantial number of derivatives are unspecified. If $r < 0$ or $r \geq 1$, the default value is used.

Linear Feasibility Tolerance

 r_1 Default = $\sqrt{\epsilon}$

Nonlinear Feasibility Tolerance

 r_2 Default = $\epsilon^{0.33}$ or $\sqrt{\epsilon}$

The default value of r_2 is $\epsilon^{0.33}$ if **Derivative Level** = 0 or 1, and $\sqrt{\epsilon}$ otherwise.

The scalars r_1 and r_2 define the maximum acceptable *absolute* violations in linear and nonlinear constraints at a ‘feasible’ point; i.e., a linear constraint is considered satisfied if its violation does not exceed r_1 , and similarly for a nonlinear constraint and r_2 . If $r_m < \epsilon$ or $r_m \geq 1$, the default value is used, for $m = 1, 2$.

On entry to the local optimizer an iterative procedure is executed in order to find a point that satisfies the linear constraints and bounds on the variables to within the tolerance r_1 . All subsequent iterates will satisfy the linear constraints to within the same tolerance (unless r_1 is comparable to the finite difference interval).

For nonlinear constraints, the feasibility tolerance r_2 defines the largest constraint violation that is acceptable at an optimal point. Since nonlinear constraints are generally not satisfied until the final iterate, the value of optional parameter **Nonlinear Feasibility Tolerance** acts as a partial termination criterion for the iterative sequence generated by the local minimizer (see the discussion of optional parameter **Optimality Tolerance**).

These tolerances should reflect the precision of the corresponding constraints. For example, if the variables and the coefficients in the linear constraints are of order unity, and the latter are correct to about 6 decimal digits, it would be appropriate to specify r_1 as 10^{-6} .

List

Nolist

Default

For nag_glopt_nlp_multistart_sqp_lsq (e05usc), normally each optional parameter specification is not printed as it is supplied. Optional parameter **Nolist** may be used to suppress the printing and optional parameter **List** may be used to turn on printing.

Major Iteration Limit

 i Default = $\max(50, 3(n + n_L) + 10n_N)$

Iteration Limit

Iters

Itns

The value of i specifies the maximum number of major iterations allowed before termination of each local subproblem. Setting $i = 0$ and **Major Print Level** > 0 means that the workspace needed by each local minimization will be computed and printed, but no iterations will be performed. If $i < 0$, the default value is used.

Major Print Level

 i

Default = 10

Print Level

 i

The value of i controls the amount of printout produced by the major iterations of nag_glopt_nlp_multistart_sqp_lsq (e05usc), as indicated below. A detailed description of the printed output is given in Section 9.1 (summary output at each major iteration and the final solution) and Section 13 (monitoring information at each major iteration). (See also the description of the optional parameter **Minor Print Level**.)

The following printout is sent to `stdout`:

i	Output
0	No output.

For the other values described below, the arguments used by the local minimizer are displayed in addition to intermediate and final output.

i	Output
1	The final solution only.
5	One line of summary output (< 80 characters; see Section 9.1) 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 file associated with the FileID defined by the optional parameter **Monitoring File**:

<i>i</i>	Output
< 5	No output.
≥ 5	One long line of output (> 80 characters; see Section 13) for each major iteration (no printout of the final solution).
≥ 20	At each major iteration, the objective function, the Euclidean norm of the nonlinear constraint violations, the values of the nonlinear constraints (the vector c), the values of the linear constraints (the vector $A_L x$), and the current values of the variables (the vector x).
≥ 30	At each major iteration, the diagonal elements of the matrix T associated with the TQ factorization (5) in nag_opt_nlp_revcomm (e04ufc) (see Section 11 in nag_opt_nlp_solve (e04wdc)) of the QP working set, and the diagonal elements of R , the triangular factor of the transformed and reordered Hessian (6) in nag_opt_nlp_revcomm (e04ufc) (see Section 11 in nag_opt_nlp_solve (e04wdc)).

Minor Iteration Limit *i* Default = $\max(50, 3(n + n_L + n_N))$

The value of i specifies the maximum number of iterations for finding a feasible point with respect to the bounds and linear constraints (if any). The value of i also specifies the maximum number of minor iterations for the optimality phase of each QP subproblem. If $i \leq 0$, 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 nag_glopt_nlp_multistart_sqplsq (e05usc) (i.e., the iterations of the quadratic programming algorithm), as indicated below. A detailed description of the printed output is given in Section 9.1 (summary output at each minor iteration and the final QP solution) and Section 13 (monitoring information at each minor iteration). (See also the description of the optional parameter **Major Print Level**.) The following printout is sent to `stdout`:

<i>i</i>	Output
0	No output.
1	The final QP solution only.
5	One line of summary output (< 80 characters; see Section 9.1) for each minor iteration (no printout of the final QP solution).
≥ 10	The final QP solution and one line of summary output for each minor iteration.

The following printout is sent to the file associated with the FileID defined by the optional parameter **Monitoring File**:

<i>i</i>	Output
< 5	No output.
≥ 5	One long line of output (> 80 characters; see Section 9.1) for each minor iteration (no printout of the final QP solution).
≥ 20	At each minor iteration, the current estimates of the QP multipliers, the current estimate of the QP search direction, the QP constraint values, and the status of each QP constraint.
≥ 30	At each minor iteration, the diagonal elements of the matrix T associated with the TQ factorization (5) in nag_opt_nlp_revcomm (e04ufc) (see Section 11 in nag_opt_nlp_solve (e04wdc)) of the QP working set, and the diagonal elements of the Cholesky factor R of the transformed Hessian (6) in nag_opt_nlp_revcomm (e04ufc) (see Section 11 in nag_opt_nlp_solve (e04wdc)).

Monitoring File Default = -1

(See Section 2.3.1.1 in How to Use the NAG Library and its Documentation for further information on NAG data types.)

i is of the type `Nag_FileID` and is obtained by a call to `nag_open_file` (x04acc).

If $i \geq 0$ and **Major Print Level** ≥ 5 or $i \geq 0$ and **Minor Print Level** ≥ 5 , monitoring information produced by `nag_glopt_nlp_multistart_sqplsq` (e05usc) at every iteration is sent to a file with ID i . If $i < 0$ and/or **Major Print Level** < 5 and **Minor Print Level** < 5 , no monitoring information is produced.

Optimality Tolerance

 r Default = $\epsilon_R^{0.8}$

The argument r ($\epsilon_R \leq r < 1$) specifies the accuracy to which you wish the final iterate to approximate a solution of each local problem. Broadly speaking, r indicates the number of correct figures desired in the objective function at the solution. For example, if r is 10^{-6} and a local minimization terminates successfully, the final value of F should have approximately six correct figures. If $r < \epsilon_r$ or $r \geq 1$, the default value is used.

The local optimizer will terminate successfully if the iterative sequence of x values is judged to have converged and the final point satisfies the first-order Kuhn–Tucker conditions (see Section 11 in `nag_opt_nlp_solve` (e04wdc)) The sequence of iterates is considered to have converged at x if

$$\alpha \|p\| \leq \sqrt{r}(1 + \|x\|), \quad (2)$$

where p is the search direction and α the step length from (3) in `nag_opt_nlp_revcomm` (e04ufc). An iterate is considered to satisfy the first-order conditions for a minimum if

$$\|Z^T g_{FR}\| \leq \sqrt{r}(1 + \max(1, |F(x)|, \|g_{FR}\|)) \quad (3)$$

and

$$|res_j| \leq ftol \quad \text{for all } j, \quad (4)$$

where $Z^T g_{FR}$ is the projected gradient (see Section 11 in `nag_opt_nlp_solve` (e04wdc)), g_{FR} is the gradient of $F(x)$ with respect to the free variables, res_j is the violation of the j th active nonlinear constraint, and $ftol$ is the **Nonlinear Feasibility Tolerance**.

Out_Level

 i

Default = 0

This option defines the amount of extra information to be sent to a file associated with **Punch Unit**. The possible choices for i are the following:

i	Meaning
-----	---------

- | | |
|---|--|
| 0 | No extra output. |
| 1 | Updated solutions only. This is useful during long runs to observe progress. |
| 2 | Successful start points only. This is useful to save the starting points that gave rise to the final solution. |
| 3 | Both updated solutions and successful start points. |

Punch Unit

 i

Default = 0

This option allows you to send information arising from an appropriate setting of **Out_Level** to be sent to a file with an integer identifier i . i must be obtained by a call to `nag_open_file` (x04acc) where i is the third argument to `nag_open_file` (x04acc).

Start Objective Check At Variable	i_1	Default = 1
Stop Objective Check At Variable	i_2	Default = n
Start Constraint Check At Variable	i_3	Default = 1
Stop Constraint Check At Variable	i_4	Default = n

These keywords take effect only if **Verify Level** > 0 . They may be used to control the verification of gradient elements computed by **objfun** and/or Jacobian elements computed by **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, it is reasonable to specify **Start Objective Check At Variable** = 31.

If the first 30 variables appear linearly in the objective, so that the corresponding gradient elements are constant, the above choice would also be appropriate.

If $i_{2m-1} \leq 0$ or $i_{2m-1} > \min(n, i_{2m})$, the default value is used, for $m = 1, 2$. If $i_{2m} \leq 0$ or $i_{2m} > n$, the default value is used, for $m = 1, 2$.

Step Limit

r

Default = 2.0

If $r > 0$, r specifies the maximum change in variables at the first step of the linesearch. 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 encourage evaluation of the problem functions at meaningful points. Given any major iterate x , the first point \tilde{x} at which F and c are evaluated during the linesearch is restricted so that

$$\|\tilde{x} - x\|_2 \leq r(1 + \|x\|_2).$$

The linesearch may go on and evaluate F and c at points further from x if this will result in a lower value of the merit function (indicated by L at the end of each line of output produced by the major iterations; see Section 9.1). If L is printed for most of the iterations, r should be set to a larger value.

Wherever possible, upper and lower bounds on x should be used to prevent evaluation of nonlinear functions at wild values. The default value **Step Limit** = 2.0 should not affect progress on well-behaved functions, but values such as 0.1 or 0.01 may be helpful when rapidly varying functions are present. If a small value of **Step Limit** 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.

Verify Level

i

Default = 0

Verify

i

Verify Constraint Gradients

i

Verify Gradients

i

Verify Objective Gradients

i

These keywords refer to finite difference checks on the gradient elements computed by **objfun** and **confun**. The possible choices for i are as follows:

i	Meaning
-1	No checks are performed.
0	Only a 'cheap' test will be performed.
≥ 1	Individual gradient elements will also be checked using a reliable (but more expensive) test.

It is possible to specify **Verify Level** = 0 to 3 in several ways. For example, the nonlinear objective gradient (if any) will be verified if either **Verify Objective Gradients** or **Verify Level** = 1 is specified. The constraint gradients will be verified if **Verify** = YES or **Verify Level** = 2 or **Verify** is specified. Similarly, the objective and the constraint gradients will be verified if **Verify** = YES or **Verify Level** = 3 or **Verify** is specified.

If $0 \leq i \leq 3$, gradients will be verified at the first point that satisfies the linear constraints and bounds.

If $i = 0$, only a 'cheap' test will be performed, requiring one call to **objfun** and (if appropriate) one call to **confun**.

If $1 \leq i \leq 3$, a more reliable (but more expensive) check will be made on individual gradient elements, within the ranges specified by the **Start Constraint Check At Variable** and **Stop Constraint Check At Variable** keywords. A result of the form OK or BAD? is printed by nag_glopt_nlp_multistart_sqp_ls (e05usc) to indicate whether or not each element appears to be correct.

If $10 \leq i \leq 13$, the action is the same as for $i = 10$, except that it will take place at the user-specified initial value of x .

If $i < -1$ or $4 \leq i \leq 9$ or $i > 13$, the default value is used.

We suggest that **Verify Level** = 3 be used whenever a new function is being developed.

13 Description of Monitoring Information

This section describes the long line of output (> 80 characters) which forms part of the monitoring information produced by `nag_glopt_nlp_multistart_sqp_lsq` (e05usc). (See also the description of the optional parameters **Major Print Level**, **Minor Print Level** and **Monitoring File**.) You can control the level of printed output.

When **Major Print Level** ≥ 5 and **Monitoring File** ≥ 0 , the following line of output is produced at every major iteration of `nag_glopt_nlp_multistart_sqp_lsq` (e05usc) on the file specified by **Monitoring File**. In all cases, the values of the quantities printed are those in effect *on completion* of the given iteration.

Maj	is the major iteration count.
Mnr	is the number of minor iterations required by the feasibility and optimality phases of the QP subproblem. Generally, Mnr will be 1 in the later iterations, since theoretical analysis predicts that the correct active set will be identified near the solution (see Section 11). 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 α_k taken along the computed search direction. On reasonably well-behaved local problems, the unit step (i.e., $\alpha_k = 1$) will be taken as the solution is approached.
Nfun	is the cumulative number of evaluations of the objective function needed for the linesearch. Evaluations needed for the estimation of the gradients by finite differences are not included. Nfun is printed as a guide to the amount of work required for the linesearch.
Merit Function	is the value of the augmented Lagrangian merit function (12) in <code>nag_opt_nlp_revcomm</code> (e04ufc) at the current iterate. This function will decrease at each iteration unless it was necessary to increase the penalty parameters (see Section 11 in <code>nag_opt_nlp_solve</code> (e04wdc)). As the solution is approached, Merit Function will converge to the value of the objective function at the solution. If the QP subproblem does not have a feasible point (signified by I at the end of the current output line) then the merit function is a large multiple of the constraint violations, weighted by the penalty parameters. During a sequence of major iterations with infeasible subproblems, the sequence of Merit Function values will decrease monotonically until either a feasible subproblem is obtained or the local optimizer terminates. Repeated failures will prevent a feasible point being found for the nonlinear constraints. If there are no nonlinear constraints present (i.e., ncnln = 0) then this entry contains Objective, the value of the objective function $F(x)$. The objective function will decrease monotonically to its optimal value when there are no nonlinear constraints.
Norm Gz	is $\ Z^T g_{FR}\ $, the Euclidean norm of the projected gradient (see Section 11 in <code>nag_opt_nlp_solve</code> (e04wdc)) Norm Gz will be approximately zero in the neighbourhood of a solution.
Violtn	is the Euclidean norm of the residuals of constraints that are violated or in the predicted active set (not printed if ncnln is zero). Violtn will be approximately zero in the neighbourhood of a solution.
Nz	is the number of columns of Z (see Section 11 in <code>nag_opt_nlp_solve</code> (e04wdc)). The value of Nz is the number of variables minus the number of constraints in the predicted active set; i.e., $Nz = n - (\text{Bnd} + \text{Lin} + \text{Nln})$.
Bnd	is the number of simple bound constraints in the predicted active set.
Lin	is the number of general linear constraints in the predicted working set.

Nln	is the number of nonlinear constraints in the predicted active set (not printed if ncnln is zero).
Penalty	is the Euclidean norm of the vector of penalty parameters used in the augmented Lagrangian merit function (not printed if ncnln is zero).
Cond H	is a lower bound on the condition number of the Hessian approximation H .
Cond Hz	is a lower bound on the condition number of the projected Hessian approximation H_Z ($H_Z = Z^T H_{FR} Z = R_Z^T R_Z$; see (6) in nag_opt_nlp_revcomm (e04ufc)). The larger this number, the more difficult the local problem.
Cond T	is a lower bound on the condition number of the matrix of predicted active constraints.
Conv	is a three-letter indication of the status of the three convergence tests (2)–(4) defined in the description of the optional parameter Optimality Tolerance . Each letter is T if the test is satisfied and F otherwise. The three tests indicate whether: <ul style="list-style-type: none"> (i) the sequence of iterates has converged; (ii) the projected gradient (Norm Gz) is sufficiently small; and (iii) the norm of the residuals of constraints in the predicted active set (Violtn) is small enough. <p>If any of these indicators is F for a successful local minimization you should check the solution carefully.</p>
M	is printed if the quasi-Newton update has been modified to ensure that the Hessian approximation is positive definite (see Section 11 in nag_opt_nlp_solve (e04wdc)).
I	is printed if the QP subproblem has no feasible point.
C	is printed if central differences have been used to compute the unspecified objective and constraint gradients. If the value of Step is zero then the switch to central differences was made because no lower point could be found in the linesearch. (In this case, the QP subproblem is resolved with the central difference gradient and Jacobian.) If the value of Step is nonzero then central differences were computed because Norm Gz and Violtn imply that x is close to a Kuhn–Tucker point (see Section 11 in nag_opt_nlp_solve (e04wdc)).
L	is printed if the linesearch has produced a relative change in x greater than the value defined by the optional parameter Step Limit . If this output occurs frequently during later iterations of the run, optional parameter Step Limit should be set to a larger value.
R	is printed if the approximate Hessian has been refactorized. If the diagonal condition estimator of R indicates that the approximate Hessian is badly conditioned then the approximate Hessian is refactorized using column interchanges. If necessary, R is modified so that its diagonal condition estimator is bounded.

When **Minor Print Level** ≥ 5 and **Monitoring File** ≥ 0 , the following line of output is produced at every minor iteration of nag_glopt_nlp_multistart_sqp_lsq (e05usc) on the file specified by **Monitoring File**. In all cases, the values of the quantities printed are those in effect *on completion* of the given iteration.

Itn	is the iteration count.
Jdel	is the index of the constraint deleted from the working set. If Jdel is zero, no constraint was deleted.
Jadd	is the index of the constraint added to the working set. If Jadd is zero, no constraint was added.

Step	is the step taken along the computed search direction. If a constraint is added during the current iteration (i.e., Jadd is positive), Step will be the step to the nearest constraint. During the optimality phase, the step can be greater than one only if the factor R_Z is singular.
Ninf	is the number of violated constraints (infeasibilities). This will be zero during the optimality phase.
Sinf/Objective	is the value of the current objective function. If x is not feasible, Sinf gives a weighted sum of the magnitudes of constraint violations. If x is feasible, Objective is the value of the objective function of the QP subproblem. The output line for the final iteration of the feasibility phase (i.e., the first iteration for which Ninf is zero) will give the value of the true objective at the first feasible point. During the optimality phase the value of the objective function will be nonincreasing. During the feasibility phase the number of constraint infeasibilities will not increase until either a feasible point is found or the optimality of the multipliers implies that no feasible point exists. Once optimal multipliers are obtained the number of infeasibilities can increase, but the sum of infeasibilities will either remain constant or be reduced until the minimum sum of infeasibilities is found.
Bnd	is the number of simple bound constraints in the current working set.
Lin	is the number of general linear constraints in the current working set.
Art	is the number of artificial constraints in the working set, i.e., the number of columns of Z_2 (see Section 11).
Zr	is the number of columns of Z_1 (see Section 11). Zr is the dimension of the subspace in which the objective function is currently being minimized. The value of Zr is the number of variables minus the number of constraints in the working set; i.e., $Zr = n - (Bnd + Lin + Art)$. The value of n_Z , the number of columns of Z (see Section 11) can be calculated as $n_Z = n - (Bnd + Lin)$. A zero value of n_Z implies that x lies at a vertex of the feasible region.
Norm Gz	is $\ Z_1^T g_{FR}\ $, the Euclidean norm of the reduced gradient with respect to Z_1 . During the optimality phase, this norm will be approximately zero after a unit step.
Norm Gf	is the Euclidean norm of the gradient function with respect to the free variables, i.e., variables not currently held at a bound.
Cond T	is a lower bound on the condition number of the working set.
Cond Rz	is a lower bound on the condition number of the triangular factor R_1 (the first Zr rows and columns of the factor R_Z). If the estimated rank of the data matrix A is zero then Cond Rz is not printed.
