User's Guide for DNOPT Version 2: Software for Nonlinear Programming*

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Abstract

DNOPT is a general-purpose system for constrained optimization. It minimizes a linear or nonlinear function subject to bounds on the variables and general linear or nonlinear constraints. It is suitable for linear and quadratic programming and for linearly constrained optimization, as well as for general nonlinear programs.

DNOPT finds solutions that are *locally optimal*, and ideally any nonlinear functions should be smooth and users should provide gradients. It is often more widely useful. For example, local optima are often global solutions, and discontinuities in the function gradients can often be tolerated if they are not too close to an optimum. Unknown gradients are estimated by finite differences.

DNOPT uses a sequential quadratic programming (SQP) algorithm. Search directions are obtained from QP subproblems that minimize a quadratic model of the Lagrangian function subject to linearized constraints. An augmented Lagrangian merit function is reduced along each search direction to ensure convergence from any starting point.

On large problems, DNOPT is most efficient if only some of the variables enter nonlinearly, or there are relatively few degrees of freedom at a solution (i.e., many constraints are active). DNOPT requires relatively few evaluations of the problem functions. Hence it is especially effective if the objective or constraint functions (and their gradients) are expensive to evaluate.

The source code is re-entrant and suitable for any machine with a Fortran compiler (or the f2c translator and a C compiler). DNOPT may be called from a driver program in Fortran, C, or MATLAB.

Keywords: optimization, nonlinear programming, nonlinear constraints, SQP methods, quasi-Newton updates, Fortran software, C software.

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1. Introduction

DNOPT is a general-purpose system for constrained optimization. It minimizes a linear or nonlinear function subject to bounds on the variables and sparse linear or nonlinear constraints. It is suitable for large-scale linear and quadratic programming and for linearly constrained optimization, as well as for general nonlinear programs of the form

where x is an n-vector of variables, l and u are constant lower and upper bounds, $f_0(x)$ is a smooth scalar objective function, A_L is a matrix, and f(x) is a vector of smooth nonlinear constraint functions $\{f_i(x)\}$. An optional parameter Maximize may specify that $f_0(x)$ should be maximized instead of minimized.

Ideally, the first derivatives (gradients) of $f_0(x)$ and $f_i(x)$ should be known and coded by the user. If only some of the gradients are known, DNOPT estimates the missing ones by finite differences.

Upper and lower bounds are specified for all variables and constraints. The jth constraint may be defined as an equality by setting $l_j = u_j$. If certain bounds are not present, the associated elements of l or u may be set to special values that are treated as $-\infty$ or $+\infty$. Free variables and free constraints ("free rows") have both bounds infinite.

1.1. Problem types

If $f_0(x)$ is linear and f(x) is absent, NP is a linear program (LP) and DNOPT applies the primal simplex method [2]. In this case, the dense orthogonal factors of a nonsingular working-set matrix are maintained.

If only the objective is nonlinear, the problem is *linearly constrained* (LC) and tends to solve more easily than the general case with nonlinear constraints (NC). For both nonlinear cases, DNOPT applies a sequential quadratic programming (SQP) method [7], using quasi-Newton approximations to the Hessian of the Lagrangian. The merit function for steplength control is an augmented Lagrangian, as in the sparse SQP solver SNOPT [8, 9].

The DNOPT package is suitable for nonlinear problems with up to several hundred constraints and variables, and is most efficient if only some of the variables enter nonlinearly, or there are relatively few degrees of freedom at a solution (i.e., many constraints are active).

1.2. Implementation

DNOPT is implemented as a library of Fortran 77 subroutines. The source code is compatible with all known Fortran 77, 90, and 95 compilers, and can be converted to C code by the f2c translator [4] included with the distribution.

All routines in DNOPT are intended to be re-entrant (as long as the compiler allocates local variables dynamically). Hence they may be used in a parallel or multi-threaded environment. They may also be called recursively.

1.3. The DNOPT interfaces

DNOPT contains several *interfaces* between the user and the underlying solver, allowing problems to be specified in various formats.

For efficiency reasons, the solver routine dnOpt (the principal interface) requires nonlinear variables and constraints to come before linear variables and constraints, and they treat nonlinear objective functions separately from nonlinear constraints.

In some applications, the objective and constraint functions share data and computation. A summary of the DNOPT interfaces follows:

dnOpt (Section 3) is the basic interface to the underlying solver. Nonlinear constraints and variables must appear first. A nonlinear objective is defined separately from any nonlinear constraints.

1.4. Files

Every DNOPT interface reads or creates some of the following files:

Print file (Section 5) is a detailed iteration log with error messages and perhaps listings of the options and the final solution.

Summary file (Section 5.7) is a brief iteration log with error messages and the final solution status. Intended for screen output in an interactive environment.

Specs file (Section 4) is a set of run-time options, input by dnSpec.

Solution file (Sections 5.5–5.6) keeps a separate copy of the final solution listing.

Unit numbers for the Specs, Print, and Summary files are defined by inputs to subroutines dnBEGIN and dnSpec. The other DNOPT files are described in Sections 5.

1.5. Overview of the package

DNOPT is normally accessed via a sequence of subroutine calls. For example, the interface dnOpt is invoked by the statements

```
call dnBEGIN( iPrint, iSumm, ... )
call dnSpec( iSpecs, ... )
call dnopt( Start, nF, n, ... )
call dnEND( Start, nF, n, ... )
```

where dnSpec reads a file of run-time options (if any). Also, individual run-time options may be "hard-wired" by calls to dnSet, dnSeti and dnSetr.

1.6. Subroutines dnBEGIN, dnEND

Calls to subroutines dnBEGIN and dnEND start and finish a run (or set of runs) for a given problem. Subroutine dnBEGIN must be called before any other DNOPT routine. It defines the Print and Summary files, prints a title on both files, and sets all user options to be undefined. (Each DNOPT interface will later check the options and set undefined ones to default values.)

```
subroutine dnBEGIN
& (iPrint, iSumm, cw, lencw, iw, leniw, rw, lenrw)
integer
& iPrint, iSumm, lencw, leniw, lenrw, iw(leniw)
character
& cw(lencw)*8
double precision
& rw(lenrw)
```

On entry:

iPrint defines a unit number for the Print file. Typically iPrint = 9.

On some systems, the file may need to be opened before dnBEGIN is called. If $iPrint \leq 0$, there will be no Print file output.

iSumm defines a unit number for the Summary file. Typically iSumm = 6. (In an interactive environment, this usually denotes the screen.)

On some systems, the file may need to be opened before dnBEGIN is called. If $iSumm \leq 0$, there will be no Summary file output.

cw(lencw), iw(leniw), rw(lenrw) must be the same arrays that are passed to other DNOPT routines. They must all have length 500 or more.

On exit:

Some elements of cw, iw, rw are given values to indicate that most optional parameters are undefined.

The calling sequence for dnEND is identical to that of dnBEGIN.

```
subroutine dnEND
& ( iPrint, iSumm, cw, lencw, iw, leniw, rw, lenrw )
integer
& iPrint, iSumm, lencw, leniw, lenrw, iw(leniw)
character
& cw(lencw)*8
double precision
& rw(lenrw)
```

2. Description of the SQP method

Here we summarize the main features of the SQP algorithm used in DNOPT and introduce some terminology used in the description of the library routines and their arguments. The SQP algorithm is fully described by Gill, Murray and Saunders [8].

2.1. Major iterations

The basic structure of the SQP algorithm involves major and minor iterations. The major iterations generate a sequence of iterates $\{x_k\}$ that satisfy the linear constraints and converge to a point that satisfies the nonlinear constraints and the first-order conditions for optimality. At each x_k a QP subproblem is used to generate a search direction toward what will be the next iterate x_{k+1} . The constraints of the subproblem are formed from the linear constraints $l_L \leq A_L x \leq u_L$ and the linearized constraint

$$l_N \le f(x_k) + f'(x_k)(x - x_k) \le u_N,$$

where $f'(x_k)$ denotes the Jacobian matrix, whose elements are the first derivatives of f(x) evaluated at x_k . The QP constraints therefore comprise the m linear constraints

$$l \le \binom{x}{Ax - b} \le u,$$

where the $m \times n$ matrix A and m-vector b are defined as

$$A = \begin{pmatrix} f'(x_k) \\ A_L \end{pmatrix}$$
 and $b = \begin{pmatrix} -f(x_k) + f'(x_k)x_k \\ 0 \end{pmatrix}$.

With these definitions, the QP subproblem can be written as

QP_k minimize
$$q(x, x_k) = g_k^T(x - x_k) + \frac{1}{2}(x - x_k)^T H_k(x - x_k)$$

subject to $l \le \binom{x}{Ax - b} \le u$,

where $q(x, x_k)$ is a quadratic approximation to a modified Lagrangian function [7]. The matrix H_k is a quasi-Newton approximation to the Hessian of the Lagrangian. A BFGS update is applied after each major iteration. If some of the variables enter the Lagrangian linearly the Hessian will have some zero rows and columns. If the nonlinear variables appear first, then only the leading n_1 rows and columns of the Hessian need be approximated, where n_1 is the number of nonlinear variables.

2.2. Minor iterations

Solving the QP subproblem is itself an iterative procedure. Here, the iterations of the QP solver QPOPT [10] form the *minor* iterations of the SQP method. QPOPT uses a reduced-Hessian active-set method implemented as a *reduced-gradient method*.

At each minor iteration, a subset of the QP constraints are satisfied with equality. The components of x are partitioned into subvectors x_{FX} and x_{FR} where x_{FX} are the components that are chosen to be equal to their upper or lower bounds. This induces a partition of the subset of the active rows

$$egin{pmatrix} I_{FX} \ A_{FR} & A_{FX} \end{pmatrix},$$

where the matrix A_{FR} has linearly independent rows. The vectors x_{FX} and x_{FR} are known as the associated fixed, and free components of x.

The term *active-set method* arises because the constraints are temporarily frozen at their upper or lower bounds, and these constraints are considered to be *active*. (In practice, x_{FX} may include variables that are frozen at values strictly *between* their bounds.) The reduced-gradient method chooses to move the variables in a direction that will improve the objective function while keeping the active constraints satisfied with equality.

At a nonoptimal feasible point x we seek a search direction p such that x + p remains on the set of active constraints yet improves the QP objective. If the new point is to be feasible, we must have $A_{FR}p_{FR} + A_{FX}p_{FX} = 0$ and $p_{FX} = 0$.

Figure 1 illustrates the feasible region for the jth pair of constraints $\ell_j \leq r_j(x) \leq u_j$. The quantity δ is the optional parameter Feasibility tolerance. The constraints $\ell_j \leq r_j \leq u_j$ are considered "satisfied" if r_j lies in Regions 2, 3 or 4, and "inactive" if r_j lies in Region 3. The constraint $r_j \geq \ell_j$ is considered "active" in Region 2, and "violated" in Region 1. Similarly, $r_j \leq u_j$ is active in Region 4, and violated in Region 5. For equality constraints $(\ell_j = u_j)$, Regions 2 and 4 are the same and Region 3 is empty.

2.3. The reduced Hessian and reduced gradient

The conditions $A_{FR}p_{FR} + A_{FX}p_{FX} = 0$ and $p_{FX} = 0$ on the components of p may be expressed compactly as $p = Zp_Z$, where Z is a matrix that spans the null space of the active constraints:

$$Z = P \binom{Z_{FR}}{0} \tag{2.1}$$

where P permutes the columns of the working-set matrix A_W into the order $(A_{FR} \ A_{FX})$. Minimizing $q(x, x_k)$ with respect to p_z now involves a quadratic function of p_z :

$$g^T\!Zp_z + \tfrac{1}{2}p_z^TZ^T\!HZp_z,$$

where g and H are expanded forms of g_k and H_k defined for all variables (x, s). This is a quadratic with Hessian Z^THZ (the reduced Hessian) and constant vector Z^Tg (the reduced gradient). If the reduced Hessian is nonsingular, p_z is computed from the system

$$Z^T H Z p_z = -Z^T g. (2.2)$$

Once p_z is specified, p is uniquely determined from the definition $p = Zp_z$. The number of components of p_z (n_z say) therefore indicates the *number of degrees of freedom* remaining after the constraints have been satisfied. In broad terms, n_z is a measure of *how nonlinear* the problem is. In particular, n_z need not be more than one for linear problems.



Figure 1: Illustration of the constraints $\ell_j \leq r_j(x) \leq u_j$. The bounds ℓ_j and u_j are considered "satisfied" if $r_j(x)$ lies in Regions 2, 3 or 4, where δ is the feasibility tolerance. The constraints $r_j(x) \geq \ell_j$ and $r_j(x) \leq u_j$ are both considered "inactive" if $r_j(x)$ lies in Region 3.

An orthogonal factorization package is used to maintain TQ factors of A_{FR} as the working set changes. A TQ factorization of A_{FR} is given by:

$$A_{FR}Q_{FR} = \begin{pmatrix} 0 & T_{FR} \end{pmatrix}, \tag{2.3}$$

where T_{FR} is a nonsingular $m_w \times m_w$ upper-triangular matrix, and Q_{FR} is an $n \times n$ nonsingular matrix constructed from a product of orthogonal transformations (see [11]). If the columns of Q_{FR} are partitioned so that

$$Q_{\scriptscriptstyle FR} = (Z_{\scriptscriptstyle FR} \quad Y_{\scriptscriptstyle FR}),$$

where $Y_{\scriptscriptstyle FR}$ is $n \times m_w$ and $Z_{\scriptscriptstyle FR}$ is $n \times n_z$ (where $n_z = n - m_w$).

The optimality conditions for subproblem QP_k may be written in terms of the vectors y_{FX} and y_{FR} that satisfy

$$\begin{pmatrix} & A_{FR}^T \\ I_{FX} & A_{FX}^T \end{pmatrix} \begin{pmatrix} y_{FX} \\ y_{W} \end{pmatrix} = \begin{pmatrix} g_{FR} \\ g_{FX} \end{pmatrix}$$

The components of y are known as the dual variables or Lagrange multipliers. The optimality conditions for subproblem QP_k may be written in terms of y. The current point is optimal if $y_j \geq 0$ for all working-set constraints at their lower bounds, $y_j \leq 0$ for all working-set constraints at their upper bounds, and $y_j = 0$ for all constraints not in the working set (y = 0). In practice, DNOPT requests an approximate QP solution $(\widehat{x}_k, \widehat{s}_k, \widehat{y}_k)$ with slightly relaxed conditions on y_j .

If y=0, no improvement can be made with the current working set, and a constraint with non-optimal dual variable is selected to be removed from the working set. The iteration is then repeated with n_z increased by one. At all stages, if the step x+p cause a constraint to be violated, a shorter step $x+\alpha p$ is taken, one of the constraints is added to the working set, and n_z is decreased by one.

With each of the rows of the QP constraint matrix

$$\begin{pmatrix} I \\ A \end{pmatrix}$$
,

we associate the component z_j of a vector z such that $z_j = 0$ the variable or constraint is not in the working set, and z_j is the component of y_A or y_{FX} if the associated constraint is in the working set.

The reduced Hessian system (2.2) is solved an upper-triangular matrix R is maintained satisfying $R^TR = Z^THZ$. Normally, R is computed from Z^THZ at the start of phase 2 and is then updated as the working set changes. For efficiency the dimension of R should not be excessive (say, $n_s \leq 1000$). This is guaranteed if the number of nonlinear variables is "moderate".

2.4. Constraints and slack variables

Problem NP contains n variables in x. Let m be the number of components of f(x) and A_Lx combined. The upper and lower bounds on those terms define the *general constraints* of the problem. DNOPT converts the general constraints to equalities by introducing a set of *slack variables* $s = (s_1, s_2, \ldots, s_m)^T$. For example, the linear constraint $5 \le 2x_1 + 3x_2 \le +\infty$ is replaced by $2x_1 + 3x_2 - s_1 = 0$ together with the bounded slack $5 \le s_1 \le +\infty$. Problem NP can be written in the equivalent form

minimize
$$f_0(x)$$

subject to $\begin{pmatrix} f(x) \\ A_L x \end{pmatrix} - s = 0, \quad l \leq \begin{pmatrix} x \\ s \end{pmatrix} \leq u.$

The general constraints become the equalities $f(x) - s_N = 0$ and $A_L x - s_L = 0$, where s_L and s_N are the *linear* and *nonlinear slacks*.

2.5. The merit function

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

$$\mathcal{M}(x, s, y) = f_0(x) - y^T (f(x) - s_N) + \frac{1}{2} (f(x) - s_N)^T D(f(x) - s_N), \tag{2.4}$$

where D is a diagonal matrix of penalty parameters $(D_{ii} \geq 0)$, and y now refers to dual variables for the nonlinear constraints in NP. If (x_k, s_k, y_k) denotes the current solution estimate and $(\hat{x}_k, \hat{s}_k, \hat{y}_k)$ denotes the QP solution, the linesearch determines a step α_k (0 < $\alpha_k \leq 1$) such that the new point

$$\begin{pmatrix} x_{k+1} \\ s_{k+1} \\ y_{k+1} \end{pmatrix} = \begin{pmatrix} x_k \\ s_k \\ y_k \end{pmatrix} + \alpha_k \begin{pmatrix} \widehat{x}_k - x_k \\ \widehat{s}_k - s_k \\ \widehat{y}_k - y_k \end{pmatrix}$$
 (2.5)

gives a sufficient decrease in the merit function (2.4). When necessary, the penalties in D are increased by the minimum-norm perturbation that ensures descent for \mathcal{M} [14]. As in NPSOL, s_N is adjusted to minimize the merit function as a function of s prior to the solution of the QP subproblem. For more details, see [12, 3].

2.6. Treatment of constraint infeasibilities

DNOPT makes explicit allowance for infeasible constraints. First, infeasible *linear* constraints are detected by solving the linear program

where e is a vector of ones, and the nonlinear constraint bounds are temporarily excluded from l and u. This is equivalent to minimizing the sum of the general linear constraint violations subject to the bounds on x. (The sum is the ℓ_1 -norm of the linear constraint violations. In the linear programming literature, the approach is called *elastic programming*.)

The linear constraints are infeasible if the optimal solution of FP has $v \neq 0$ or $w \neq 0$. DNOPT then terminates without computing the nonlinear functions.

Otherwise, all subsequent iterates satisfy the linear constraints. (Such a strategy allows linear constraints to be used to define a region in which the functions can be safely evaluated.) DNOPT proceeds to solve NP as given, using search directions obtained from the sequence of subproblems QP_k .

If a QP subproblem proves to be infeasible or unbounded (or if the dual variables y for the nonlinear constraints become large), DNOPT enters "elastic" mode and thereafter solves the problem

where γ is a nonnegative parameter (the *elastic weight*), and $f_0(x) + \gamma e^T(v + w)$ is called a *composite objective* (the ℓ_1 penalty function for the nonlinear constraints).

The value of γ may increase automatically by multiples of 10 if the optimal v and w continue to be nonzero. If γ is sufficiently large, this is equivalent to minimizing the sum of the nonlinear constraint violations subject to the linear constraints and bounds. A similar ℓ_1 formulation of NP is fundamental to the S ℓ_1 QP algorithm of Fletcher [5]. See also Conn [1].

The initial value of γ is controlled by the optional parameter Elastic weight (p. 36).

3. The dnOpt interface

dnOpt is the principal user interface in the DNOPT package. The optimization problem is assumed to be in the form NP (p. 3) with the data ordered so that nonlinear constraints and variables come first.

A typical invocation of dnOpt is

```
call dnBEGIN( iPrint, iSumm, ... )
call dnSpec ( iSpecs, ... )
call dnopt ( n, nlCon, nnCon, ... )
call dnEND ( iPrint, iSumm, ... )
```

where dnSpec reads a set of optional parameter definitions from the file with unit number iSpecs.

3.1. Subroutines used by dnOpt

dnOpt is accessed via the following routines:

```
dnBEGIN (Section 1.6) must be called before any other dnOpt routines.
dnSpec (Section 4.4) may be called to input a Specs file (a list of run-time options).
dnSet, dnSetInt, dnSetReal (Section 4.5) may be called to specify a single option.
dnGet, dnGetChar, dnGetInt, dnGetReal (Section 4.6) may be called to obtain an option's current value.
dnOpt (Section 3.4) is the main solver.
funcon, funobj (Section 3.5) are supplied by the user and called by dnOpt. They define the constraint functions f(x) and objective function f<sub>0</sub>(x) and ideally their gradients. (They have a fixed parameter list but may have any convenient name. They are passed to dnOpt as parameters.)
dnMem computes the size of the workspace arrays iw and rw required for given problem
```

3.2. Identifying structure in the objective and constraints

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

dimensions. Intended for Fortran 90 drivers that reallocate workspace if necessary.

```
minimize (u+v+w)^2 + 3w + 5z

subject to u^2 + v^2 + w = 2

v^4 + z = 4

2u + 4v \ge 0
```

with bounds $w \ge 0$, $z \ge 0$. This problem has several characteristics that can be exploited:

- The objective function is the sum of a *nonlinear* function of the three variables x' = (u, v, w) and a *linear* function of (potentially) all variables x.
- The first two constraints are nonlinear, and the third constraint is linear.
- Each nonlinear constraint involves the sum of a *nonlinear* function of the two variables x'' = (u, v) and a *linear* function of the remaining variables y'' = (w, z).

The nonlinear terms are defined by user-written subroutines funobj and funcon, which involve only x' and x'', the appropriate subsets of variables.

For the objective, we define the function $f_0(u,v,w)=(u+v+w)^2$ to include only the nonlinear terms. The variables x'=(u,v,w) are known as nonlinear objective variables, and their dimension n'_1 is specified by the dnOpt input parameter nnObj (= 3 here). The linear part 3w+5z of the objective is treated as an additional linear constraint whose row index is specified by the input parameter iObjA. Thus, the full objective has the form $f_0(x')+d^Tx$, where x' is the first nnObj variables, $f_0(x')$ is defined by subroutine funobj, and d is a constant vector that forms row iObjA of the linear constraint matrix. Choosing iObjA = 2, we think of the problem as

minimize
$$u,v,w,z,s_4$$
 subject to
$$u^2 + v^2 + w = 2$$

$$v^4 + z = 4$$

$$2u + 4v \geq 0$$

$$3w + 5z = s_4$$

with bounds $w \ge 0$, $z \ge 0$, $-\infty \le s_4 \le \infty$, where s_4 is treated *implicitly* as the value of the 4th constraint.

Similarly for the constraints, we define a vector function f(u,v) to include just the nonlinear terms. In this example, $f_1(u,v) = u^2 + v^2$ and $f_2(u,v) = v^4$. The number of nonlinear constraints (the dimension of f) is specified by the input parameter nnCon = 2. The variables x'' = (u,v) are known as nonlinear Jacobian variables, with dimension n_1'' specified by nnJac = 2. Thus, the combined vector of nonlinear and linear constraint functions has the form

$$\begin{pmatrix} f(x'') + J_2 y'' \\ A_1 x'' + A_2 y'' \end{pmatrix}, \tag{3.1}$$

where x'' is the first nnJac variables, f(x'') is defined by subroutine funcon, and y'' contains the remaining variables, i.e., y'' = (w, z) in the example. The nonlinear and linear Jacobian matrices are then $(f'(x'') \ J_2)$ and $(A_1 \ A_2)$, and the matrix seen by the QP subproblem has the form

$$\begin{pmatrix} f'(x'') & J_2 \\ A_1 & A_2 \end{pmatrix}, \tag{3.2}$$

with the Jacobian of f always appearing in the *top left corner*. The matrices f'(x'') and J_2 are held in the array parameter JCon. The elements of JCon corresponding to f'(x'') may be given any value (the correct values are computed internally). The arrays A_1 and A_2 are input via the array parameter A. (Elements that are identically zero must be included.)

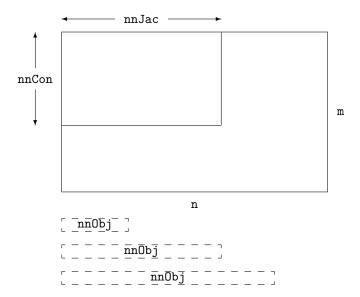
The inequalities $l_1 \leq f(x'') + J_2 y'' \leq u_1$ and $l_2 \leq A_1 x + A_2 y'' \leq u_2$ implied by the constraint functions (3.1) are known as the *nonlinear* and *linear* constraints respectively. Together, these two sets of inequalities constitute the *general constraints*.

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

Together the nonlinear objective and nonlinear Jacobian variables comprise the *nonlinear* variables. The number of nonlinear variables n_1 is therefore the *larger* of the dimensions of x' and x'', i.e., $n_1 = \max\{n'_1, n''_1\}$ (= $\max(\text{nn0bj,nnJac})$).

3.3. Problem dimensions

The following picture illustrates the problem structure just described:



The dimensions are all input parameters to subroutine dnopt (see the next section). For linear programs, nnCon, nnJac, nnObj are all zero. If a linear objective term exists, iObjA points to one of the rows of A.

The dashed boxes indicate that a nonlinear objective function $f_0(x')$ may involve either a subset or a superset of the variables in the nonlinear constraint functions f(x''), counting from the left. Thus, $nnObj \leq nnJac$ or vice versa.

Sometimes the objective and constraints really involve disjoint sets of nonlinear variables. We then recommend ordering the variables so that $\mathtt{nn0bj} > \mathtt{nnJac}$ and x' = (x'', x'''), where the objective is nonlinear in just the last vector x'''. Subroutine funobj should set $\mathtt{g0bj}(j) = 0.0$ for $j = 1:\mathtt{nnJac}$. It should then set as many remaining gradients as possible—preferably all!

3.4. Subroutine dnOpt

n

ldA ldJ

ldH

In the following specification of dnOpt, we define r(x) as the vector of combined constraint functions $r(x) = (x f(x) A_L x)$, and use nb to denote a variable that holds its dimension: nb = n + nlCon + nnCon. Note that most machines use double precision declarations as shown, but some machines use real. The same applies to the user routines funcon and funobj.

```
subroutine dnopt
          ( start, n, nlCon, nnCon, nnJac, nnObj,
            problemName, Names, nNames, iObjA, objAdd,
     г.
            funcon, funobj,
            state, A, ldA, bl, bu,
     &
            fObj, gObj, fCon, JCon, ldJ, H, ldH,
     &
            objNP, nInf, sInf, x, y,
            INFO, mincw, miniw, minrw,
     &
            cu, lencu, iu, leniu, ru, lenru,
            cw, lencw, iw, leniw, rw, lenrw)
     Хr.
      external
            funcon, funobj
      integer
     &
            iObjA, INFO, ldA, ldJ, ldH, lencw, leniw, lenrw, lencu,
     &
            leniu, lenru, n, nlCon, nnCon, nnJac, nnObj, nNames, nInf,
            mincw, miniw, minrw, start, state(n+nnCon+nlCon), iu(leniu),
     г.
            iw(leniw)
     Хr.
      double precision
            objAdd, objNP, fObj, sInf, A(ldA,*), bl(n+nnCon+nlCon),
     г.
     г.
            bu(n+nnCon+nlCon), gObj(n), fCon(ldJ), JCon(ldJ,*), H(ldH,*),
     &
            x(n+nnCon+nlCon), y(n+nnCon+nlCon), ru(lenru), rw(lenrw)
            problemName*8, Names(nNames)*8, cu(lencu)*8, cw(lencw)*8
     &
On entry:
Start is an integer that specifies how a starting point is to be obtained.
                   (Cold start) requests that a the crash procedure be used to define an
       Start = 0
                    initial working set.
       Start = 1
                   (Warm start) means that state defines a valid starting point (perhaps
                    from an earlier call, though not necessarily).
       is n, the number of variables in the problem (n > 0).
       is m_L, the number of general linear constraints (nlCon > 0).
nlCon
       is m_N, the number of nonlinear constraints (nnCon > 0).
nnCon
       is the row dimension of the array A (1dA \ge 1, 1dA \ge nlCon).
       is the row dimension of the array JCon (ldJ \ge 1, ldJ \ge nnCon).
       is the row dimension of the array Hess (1dH \ge n).
       is the number of column and row names provided in the character array Names. If
```

nName = 1, there are no names. Generic names will be used in the printed solution.

Otherwise, nName = n + m and all names must be provided.

- nnCon is m_1 , the number of nonlinear constraints. (nnCon ≥ 0)
- nnObj is n'_1 , the number of nonlinear objective variables. (nnObj ≥ 0)
- nnJac is n_1'' , the number of nonlinear Jacobian variables. If nnCon = 0, then nnJac = 0. If nnCon > 0, then nnJac > 0.
- iObjA says which row of A is a free row containing a linear objective vector c. If there is no such row, iObjA = 0.
- ObjAdd is a constant that will be added to the objective for printing purposes. Typically ObjAdd = 0.0d+0.
- ProblemName is an 8-character name for the problem. ProblemName is used in the printed solution. A blank name may be used.
- Names (nName) sometimes contains 8-character names for the variables and constraints. If nName = 1, Names is not used. The printed solution will use generic names for the columns and row. If nName = n + m, Names (j) should contain the 8-character name of the jth variable (j = 1: n + m). If j = n + i, the jth variable is the ith row.
- A is an array of dimension (1dA,k) for some $k \ge n$. It contains the matrix A_L for the linear constraints. If nlCon = 0, A is not referenced. (In that case, A may be dimensioned (1dA,1) with ldA = 1, or it could be any convenient array.)
- bl(nb), bu(nb) contain the lower and upper bounds for r(x) in problem NP.

To specify non-existent bounds, set $bl(j) \leq -\inf Bnd$ or $bu(j) \geq \inf Bnd$, where $\inf Bnd$ is the Infinite Bound size (default value 10^{20}).

To specify an equality constraint (say $r_j(x) = \beta$), set $bl(j) = bu(j) = \beta$, where $|\beta| < infBnd$.

For the data to be meaningful, it is required that $bl(j) \leq bu(j)$ for all j.

- funcon is the name of a subroutine that calculates the vector of nonlinear constraint functions f(x) and (optionally) its Jacobian for a specified vector x (the first nnJac elements of $\mathbf{x}(*)$). funcon must be declared external in the routine that calls dnOpt. For a detailed description of funcon, see Section 3.6.
- funobj is the name of a subroutine that calculates the objective function $f_0(x)$ and (optionally) its gradient for a specified vector x (the first nn0bj elements of x(*)). funobj must be declared external in the routine that calls dn0pt. For a detailed description of funobj, see Section 3.7.

For start = 1 (a warm start) every element of state must be set. If dnOpt has just been called on a problem with the same dimensions, state already contains valid values. Otherwise, state(j) should indicate whether either of the constraints $r_j(x) \ge l_j$ or $r_j(x) \le u_j$ is expected to be active at a solution of (NP).

The ordering of state is the same as for bl, bu and r(x), i.e., the first n components of state refer to the upper and lower bounds on the variables, the next nlCon refer to the bounds on $A_L x$, and the last nnCon refer to the bounds on f(x). Possible values for state(j) follow.

- Neither $r_j(x) \ge l_j$ nor $r_j(x) \le u_j$ is expected to be active.
- 1 $r_j(x) \ge l_j$ is expected to be active.

- $r_i(x) \le u_i$ is expected to be active.
- This may be used if $l_j = u_j$. Normally an equality constraint $r_j(x) = l_j = u_j$ is active at a solution.

The values 1, 2 or 3 all have the same effect when $\mathfrak{bl}(j) = \mathfrak{bu}(j)$. If necessary, dnOpt will override the user's specification of state, so that a poor choice will not cause the algorithm to fail.

JCon(ldJ,*) is an array of dimension (ldJ,k) for some $k \ge n$. If nnCon = 0, JCon is not referenced. (In that case, JCon may be dimensioned (ldJ,1) with ldJ = 1.)

In general, JCon need not be initialized before the call to dnOpt. However, if Derivative level = 3, any constant elements of JCon may be initialized. Such elements need not be reassigned on subsequent calls to funcon (see Section 3.9).

y(nb) is an array that need not be initialized if dnOpt is called with a Cold start (the default).

Otherwise, the ordering of y is the same as for bl, bu and state. For a Warm start, the components of y corresponding to nonlinear constraints must contain a multiplier estimate. The sign of each multiplier should match state as follows. If the *i*th nonlinear constraint is defined as "inactive" via the initial value $\mathtt{state}(j) = 0$, $j = \mathtt{n} + \mathtt{nlCon} + i$, then $\mathtt{y}(j)$ should be zero. If the constraint $r_j(x) \geq l_j$ is active $(\mathtt{state}(j) = 1)$, $\mathtt{y}(j)$ should be non-negative, and if $r_j(x) \leq u_j$ is active $(\mathtt{state}(j) = 2)$, $\mathtt{y}(j)$ should be non-positive.

If necessary, dnOpt will change y to match these rules.

- Hess(1dH,*) is an array of dimension (1dH,k) for some $k \geq n$. Hess need not be initialized if dnOpt is called with a Cold Start (the default), and will be taken as the identity. For a warm start, Hess provides the initial approximation of the Hessian of the Lagrangian, i.e., $H(i,j) \approx \partial^2 l(x,y)/\partial x_i \partial x_j$, where $L(x,y) = f_0(x) f(x)^T y$ and y is an estimate of the optimal Lagrange multipliers. Hess must be a positive-definite matrix.
- x(nb) usually contains a set of initial values for x or (x, s).
 - 1. For Cold starts (Start = 0), the first n elements of state and x must be defined.

If there is no wish to provide special information, you may set $\mathtt{state}(j) = 0$, $\mathtt{x}(j) = 0.0$ for all j = 1:n. All variables will be eligible for the initial working set

Less trivially, to say that the optimal value of variable j will probably be equal to one of its bounds, set $\mathtt{state}(j) = 1$ and $\mathtt{x}(j) = \mathtt{bl}(j)$ or $\mathtt{state}(j) = 2$ and $\mathtt{x}(j) = \mathtt{bu}(j)$ as appropriate.

A CRASH procedure is used to select an working set.

- 2. For Warm starts (Start = 1), all of state(1:nb) must be 0, 1 or 2 and all of x(1:nb) must have values (perhaps from some previous call).
- y contains an estimate of the vector of Lagrange multipliers for the constraints. The first nnCon components must be defined. If nothing is known about the multipliers, set y(i) = 0.0, i = 1:nnCon.
- cu(lencu), iu(leniu), ru(lenru) are 8-character, integer and real arrays of user workspace. They may be used to pass data or workspace to your function routines

funcon and funobj (which have the same parameters). They are not touched by dnOpt.

If the function routines don't reference these parameters, you may use any arrays of the appropriate type, such as cw, iw, rw (see next paragraph). Conversely, you should use the latter arrays if funcon and funobj need to access dnOpt's workspace.

cw(lencw), iw(leniw), rw(lenrw) are 8-character, integer and real arrays of workspace for dnOpt. Their lengths lencw, leniw, lenrw must all be at least 500.

In general, lencw = 500 is appropriate, but leniw and lenrw should be as large as possible because it is uncertain how much storage will be needed for the basis factorization. As an estimate, leniw should be about $10 \times \texttt{nb}$ or larger, and lenrw should be about $20 \times \texttt{nb}$ or larger.

Appropriate values may be obtained from a preliminary run with lencw = leniw = lenrw = 500. See mincw, miniw, minrw below (on exit).

On exit:

INFO reports the result of the call to dnOpt. Here is a summary of possible values. Further details are in Section 5.4.

Finished successfully

- 1 optimality conditions satisfied
- 2 feasible point found
- 3 requested accuracy could not be achieved

The problem appears to be infeasible

- 11 infeasible linear constraints
- 12 infeasible linear equalities
- 13 nonlinear infeasibilities minimized
- 14 infeasibilities minimized

The problem appears to be unbounded

- 21 unbounded objective
- 22 constraint violation limit reached

 $Resource\ limit\ error$

- 31 iteration limit reached
- 32 major iteration limit reached
- 33 the superbasics limit is too small

41 42 43	Terminated after numerical difficulties current point cannot be improved singular working set cannot satisfy the general constraints
51 52 53	Error in the user-supplied functions incorrect objective derivatives incorrect constraint derivatives the QP Hessian is indefinite
61 62 63	Undefined user-supplied functions undefined function at the first feasible point undefined function at the initial point unable to proceed into undefined region
71 72 73 74	User requested termination terminated during function evaluation terminated during constraint evaluation terminated during objective evaluation terminated from monitor routine
81 82 83 84	Insufficient storage allocated work arrays must have at least 500 elements not enough character storage not enough integer storage not enough real storage
91	Input arguments out of range invalid input argument

iter is the number of major iterations performed.

state describes the status of the constraints $l \leq r(x) \leq u$ in problem (NP). For the jth lower or upper bound, j=1 to nb, the possible values of $\mathtt{state}(j)$ are as follows, where δ is the specified Feasibility tolerance:

- -2 (Region 1) The lower bound is violated by more than δ .
- -1 (Region 5) The upper bound is violated by more than δ .
 - 0 (Region 3) Both bounds are satisfied by more than δ .
 - 1 (Region 2) The lower bound is active (to within δ).
 - 2 (Region 4) The upper bound is active (to within δ).
 - 3 (Region 2 = Region 4) The bounds are equal and the equality constraint is satisfied (to within δ).

These values of state are labeled in the printed solution as follows:

Region	1	2	3	4	5	$2 \equiv 4$
state(j)	-2	1	0	2	-1	3
Printed solution		LL	FR	UL	++	EQ

- fCon is an array of dimension at least nnCon. If nnCon = 0, fCon is not accessed, and may then be declared to be of dimension (1), or the actual parameter may be any convenient array. If nnCon > 0, fCon contains the values of the nonlinear constraint functions $f_i(x)$, i = 1: nnCon, at the final iterate.
- JCon contains the Jacobian matrix of the nonlinear constraints at the final iterate, i.e., JCon(i, j) contains the partial derivative of the *i*th constraint function with respect to the *j*th variable, i = 1: nnCon, j = 1: n. (See the discussion of JCon under funcon in Section 3.6.)
- y contains the QP multipliers from the last QP subproblem. y(j) should be non-negative if state(j) = 1 and non-positive if state(j) = 2.
- fObj is the value of the objective $f_0(x)$ at the final iterate.
- gObj(n) contains the objective gradient (or its finite-difference approximation) at the final iterate.

Hess(1dH,*) contains an estimate of H, the Hessian of the Lagrangian at x.

- x contains the final estimate of the solution.
- nInf, sInf give the number and the sum of the infeasibilities of constraints that lie outside their bounds by more than the Minor feasibility tolerance before the solution is unscaled.

If any linear constraints are infeasible, x minimizes the sum of the infeasibilities of the linear constraints subject to the upper and lower bounds being satisfied. In this case nInf gives the number of components of A_Lx lying outside their bounds. The nonlinear constraints are not evaluated.

Otherwise, x minimizes the sum of the infeasibilities of the *nonlinear* constraints subject to the linear constraints and upper and lower bounds being satisfied. In this case nInf gives the number of components of f(x) lying outside their bounds by more than the Minor feasibility tolerance. Again this is before the solution is unscaled.

Obj is the final value of the nonlinear part of the objective function. If nInf = 0, Obj is the nonlinear objective, if any. If nInf > 0 but the linear constraints are feasible, then Obj is the nonlinear objective. If nInf > 0 and the linear constraints are infeasible, Obj is zero.

Note that Obj does not include contributions from the constant term ObjAdd or the objective row, if there is one. The final value of the objective being optimized is ObjAdd + x(n+iObj) + Obj, where iObj is the index of the objective row in A.

mincw, miniw, minrw say how much character, integer, and real storage is needed to solve the problem. If Print level > 0, these values are printed. If dnOpt terminates because of insufficient storage (INFO = 82, 83 or 84), the values may be used to define better values of lencw, leniw or lenrw.

If INFO = 82, the work array cw(lencw) was too small. dnOpt may be called again with lencw = mincw.

If INFO = 83 or 84, the work arrays iw(leniw) or rw(lenrw) are too small. dnOpt may be called again with leniw or lenrw suitably larger than miniw or minrw. (The bigger the better because it is not certain how much storage the basis factorization needs.)

3.5. User-supplied subroutines for dnOpt

The user must provide subroutines to define the nonlinear parts of the objective function and nonlinear constraints. They are passed to dnOpt as external parameters funobj and funcon. (A dummy subroutine must be provided if the objective or constraints are purely linear.)

Be careful when coding the call to dnOpt: the parameters are ordered alphabetically as funcon, funobj. The first call to each function routine is also in that order.

In general, these subroutines should return all function and gradient values on every entry except perhaps the last. This provides maximum reliability and corresponds to the default setting, Derivative level = 3.

In practice it is often convenient not to code gradients. dnOpt is able to estimate gradients by finite differences, by making a call to funcon or funobj for each variable x_j whose partial derivatives need to be estimated. However, this reduces the reliability of the optimization algorithms, and it can be very expensive if there are many such variables x_j .

As a compromise, dnOpt allows you to code as many gradients as you like. This option is implemented as follows. Just before a function routine is called, each element of the gradient array is initialized to a specific value. On exit, any element retaining that value must be estimated by finite differences.

Some rules of thumb follow.

- 1. For maximum reliability, compute all function and gradient values.
- 2. If the gradients are expensive to compute, specify Nonderivative linesearch and use the input parameter mode to avoid computing them on certain entries. (Don't compute gradients if mode = 0.)
- 3. If not all gradients are known, you must specify Derivative level ≤ 2 . You should still compute as many gradients as you can. (It often happens that some of them are constant or even zero.)
- 4. Again, if the known gradients are expensive, don't compute them if mode = 0.
- 5. Use the input parameter status to test for special actions on the first or last entries.
- 6. While the function routines are being developed, use the Verify option to check the computation of gradient elements that are supposedly known. The Start and Stop options may also be helpful.
- 7. The function routines are not called until the linear constraints and bounds on x are satisfied. This helps confine x to regions where the nonlinear functions are likely to be defined. However, be aware of the Minor feasibility tolerance if the functions have singularities near bounds.
- 8. Set mode = -1 if some of the functions are undefined. The linesearch will shorten the step and try again.
- 9. Set mode ≤ -2 if you want dnOpt to stop.

3.6. Subroutine funcon

This subroutine must compute the nonlinear constraint functions $\{f_i(x)\}$ and (optionally) their derivatives. (A dummy subroutine funcon must be provided if there are no nonlinear constraints.) The *i*th row of the Jacobian JCon is the vector $(\partial f_i/\partial x_1, \partial f_i/\partial x_2, \ldots, \partial f_i/\partial x_n)$.

```
subroutine funcon
& ( mode, nnCon, nnJac, x, fCon, JCon, ldJ, status,
& cu, lencu, iu, leniu, ru, lenru )

integer
& ldJ, mode, nnCon, nnJac, status, lencu, leniu, lenru,
& iu(leniu)
double precision
& x(nnJac), fCon(nnCon), JCon(ldJ,*), ru(lenru)
character*8
& cu(lencu)
```

On entry:

mode indicates whether fCon or JCon or both must be assigned during the present call of funcon $(0 \le mode \le 2)$.

This parameter can be ignored if Perivative linesearch is selected (the default) and if Perivative level = 2 or 3. In this case, mode will always have the value 2, and all elements of Perivative level = 2 or 3. In this case, mode will always have the value 2, and all elements of Perivative level = 2 or 3. In this case, mode will always have the value 2, and all elements of Perivative level = 2 or 3.

Otherwise, dnOpt will call funcon with mode = 0, 1 or 2. You may test mode to decide what to do:

- If mode = 2, assign fCon and the known components of JCon.
- If mode = 1, assign the known components of JCon. fCon is ignored.
- If mode = 0, only fCon need be assigned; JCon is ignored.

nnCon is the number of nonlinear constraints (nnCon > 0). These must be the first nnCon constraints in the problem.

nnJac is the number of variables involved in f(x) ($0 < \text{nnJac} \le n$). These must be the first nnJac variables in the problem.

x(nnJac) contains the nonlinear Jacobian variables x. The array x must not be altered. status indicates the first and last calls to funcon.

If status = 0, there is nothing special about the current call to funcon.

If status = 1, dnOpt is calling your subroutine for the *first* time. Some data may need to be input or computed and saved. Note that if there is a nonlinear objective, the first call to funcon will occur *before* the first call to funobj.

If $status \ge 2$, dnOpt is calling your subroutine for the *last* time. You may wish to perform some additional computation on the final solution. Note again that the last call to funcon will occur *before* the last call to funobj.

In general, the last call is made with status = 2 + INFO/10, where INFO is the integer returned by dnOpt (see p. 18). In particular,

```
if status = 2, the current x is optimal; if status = 3, the problem appears to be infeasible; if status = 4, the problem appears to be unbounded; if status = 5, an iterations limit was reached.
```

If the functions are expensive to evaluate, it may be desirable to do nothing on the last call. The first executable statement could be if (status .ge. 2) return.

cu(lencu), iu(leniu), ru(lenru) are the character, integer and real arrays of user workspace provided to dnOpt. They may be used to pass information into the function routines and to preserve data between calls.

In special applications the functions may depend on some of the internal variables stored in dnOpt's workspace arrays cw, iw, rw. For example, the 8-character problem name ProblemName is stored in cw(51), and the dual variables for the general constraints are stored in rw(1yCon) onward, where lyCon = iw(268). These will be accessible to both funcon and funobj if dnOpt is called with parameters cu, iu, ru the same as cw, iw, rw.

If you still require user workspace, elements rw(501:maxru) and rw(maxrw+1:lenru) are set aside for this purpose, where maxru = iw(2). Similarly for workspace in cw and rw. (See the Total and User workspace options.)

On exit:

fCon(nnCon) contains the computed constraint vector f(x) (except perhaps if mode = 1).

JCon(nnCon,nnJac) contains the computed Jacobian f'(x) (except perhaps if mode = 0). These gradient elements must not include the elements of J_2 . There is no internal check for consistency (except indirectly via the Verify option), so great care is essential.

mode may be used to indicate that you are unable to evaluate f or its gradients at the current x. (For example, the problem functions may not be defined there).

During the linesearch, f(x) is evaluated at points $x = x_k + \alpha p_k$ for various steplengths α , where $f(x_k)$ has already been evaluated satisfactorily. For any such x, if you set mode = -1, dnOpt will reduce α and evaluate f again (closer to x_k , where it is more likely to be defined).

If for some reason you wish to terminate the current problem, set $mode \leq -2$.

3.7. Subroutine funobj

This subroutine must calculate the objective function $f_0(x)$ and (optionally) the gradient g(x).

```
subroutine funobj
& ( mode, nn0bj, x, f0bj, g0bj, status,
& cu, lencu, iu, leniu, ru, lenru )
integer
& mode, nn0bj, status, lencu, leniu, lenru, iu(leniu)
double precision
& f0bj, x(nn0bj), g0bj(nn0bj), ru(lenru)
character*8
& cu(lencu)
```

On entry:

mode may be set as in funcon.

nnObj is the number of variables involved in $f_0(x)$ ($0 < \text{nnObj} \le n$). These must be the first nnObj variables in the problem.

x(nnObj) contains the nonlinear objective variables x. The array x must not be altered. status is used as in funcon.

cu(lencu), iu(leniu), ru(lenru) are the same as in funcon.

On exit:

mode may be set as in funcon to indicate that you are unable to evaluate f_0 at x.

If you wish to terminate the solution of the current problem, set mode ≤ -2 .

fObj must contain the computed value of $f_0(x)$ (except perhaps if mode = 1).

gObj(nnObj) must contain the known components of the gradient vector g(x), i.e., gObj(j) contains the partial derivative $\partial f_0/\partial x_i$ (except perhaps if mode = 0).

3.8. Example

Here we give the subroutines funobj and funcon for the example of Section 3.2, repeated here for convenience with generic variables x_i :

minimize
$$(x_1 + x_2 + x_3)^2 + 3x_3 + 5x_4$$

subject to $x_1^2 + x_2^2 + x_3 = 2$
 $x_2^4 + x_4 = 4$
 $2x_1 + 4x_2 \ge 0$

and $x_3 \ge 0$, $x_4 \ge 0$. This problem has 4 variables, 3 nonlinear objective variables, 2 nonlinear Jacobian variables, 2 nonlinear constraints, 1 linear constraint, and two bounded variables. The objective has some linear terms that we include as an extra "free row" (with infinite bounds). The calling program must assign the following values:

```
n = 4 nlCon = 2 nnCon = 2 nnObj = 3 nnJac = 2 iObjA = 2
```

Subroutine funobj works with the nonlinear objective variables (x_1, x_2, x_3) . As x_3 occurs only linearly in the constraints, we have placed it *after* the Jacobian variables (x_1, x_2) .

For interest, we test mode to economize on gradient evaluations (even though they are cheap here). Note that Nonderivative linesearch would have to be specified, otherwise all entries would have mode = 2.

```
subroutine funobj
& ( mode, nn0bj, x, f0bj, g0bj, Status,
& cu, lencu, iu, leniu, ru, lenru )

integer
& mode, nn0bj, Status, lencu, leniu, lenru, iu(leniu)
double precision
& f0bj, x(nn0bj), g0bj(nn0bj), ru(lenru)
character*8
& cu(lencu)
```

```
_____
Simple toy Problem.
_____
double precision
 sum
sum = x(1) + x(2) + x(3)
if (mode .eq. 0 .or. mode .eq. 2) then
 fObj
      = sum*sum
end if
if (mode .eq. 1 .or. mode .eq. 2) then
  sum = 2.0d+0*sum
  gObj(1) = sum
 gObj(2) = sum
  gObj(3) = sum
end if
end ! subroutine funobj
```

Subroutine funcon involves only (x_1, x_2) . First we treat the Jacobian as a *dense matrix*. In Fortran it is preferable to access two-dimensional arrays column-wise, as shown. Each column of gCon contains two elements, even though one of them is zero. The Acol, indA, locA data structure *must include these elements*, as well as other entries belonging to the linear constraints.

As funcon is called before funobj, we test status for the first and last entries.

```
subroutine funcon
      ( mode, nnCon, nnJac, x, fCon, JCon, ldJ, status,
        cu, lencu, iu, leniu, ru, lenru)
    integer
        ldJ, mode, nnCon, nnJac, status, lencu, leniu, lenru,
        iu(leniu)
    double precision
        x(nnJac), fCon(nnCon), JCon(ldJ,*), ru(lenru)
    character*8
        cu(lencu)
    ______
    Simple toy Problem.
    _____
    integer
                   Out
    parameter
                 (Out = 6)
    ______
    Print something on the first and last entry.
    if (status .eq. 1) then
                            ! First
      if (Out .gt. 0) write(Out, '(/a)') 'Starting dntoy'
    else if (status .ge. 2) then ! Last
       if (Out .gt. 0) write(Out, '(/a)') 'Finishing dntoy'
      return
    end if
    if (mode .eq. 0 .or. mode .eq. 2) then
      fCon(1) = x(1)**2 + x(2)**2
      fCon(2) =
    end if
    if (mode .ge. 1) then
ı
!
      Nonlinear elements for row 1
       ______
      JCon(1,1) = 2.0d+0*x(1)
      JCon(1,2) = 2.0d+0*x(2)
      Nonlinear elements for row 2
      JCon(2,2) = 4.0d+0*x(2)**3
    end if
```

end ! subroutine funcon

3.9. Constant Jacobian elements

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

Note that constant *nonzero* elements do affect the values of the constraints. Thus, if $\mathsf{JCon}(i,j)$ is set to a constant value, it need not be reset in subsequent calls to funcon , but the value $\mathsf{JCon}(i,j)*x(j)$ must nonetheless be added to $\mathsf{fCon}(i)$.

It must be emphasized that, if Derivative level < 2, unassigned elements of JCon are not treated as constant; they are estimated by finite differences, at non-trivial expense.

4. Optional parameters

The performance of each DNOPT interface is controlled by a number of parameters or "options". Each option has a default value that should be appropriate for most problems. Other values may be specified in two ways:

- By calling subroutine dnSpec to read a Specs file (Section 4.1).
- By calling the option-setting routines dnSet, dnSetInt, dnSetReal (Section 4.5).

The current value of an optional parameter may be examined by calling one of the routines dnGet, dnGetChar, dnGetInt, dnGetReal (Section 4.6).

4.1. The SPECS file

The Specs file contains a list of options and values in the following general form:

```
Begin options
Iterations limit 500
Minor feasibility tolerance 1.0e-7
Solution Yes
End options
```

We call such data a Specs file because it specifies various options. The file starts with the keyword Begin and ends with End. The file is in free format. Each line specifies a single option, using one or more items as follows:

- 1. A keyword (required for all options).
- 2. A phrase (one or more words) that qualifies the keyword (only for some options).
- 3. A *number* that specifies an integer or real value (only for some options). Such numbers may be up to 16 contiguous characters in Fortran 77's I, F, E or D formats, terminated by a space or new line.

The items may be entered in upper or lower case or a mixture of both. Some of the keywords have synonyms, and certain abbreviations are allowed, as long as there is no ambiguity. Blank lines and comments may be used to improve readability. A comment begins with an asterisk (*) anywhere on a line. All subsequent characters on the line are ignored.

The Begin line is echoed to the Summary file.

4.2. Multiple sets of options in the Specs file

The keyword Skip allows you to collect several sets of options within a single Specs file. In the following example, only the second set of options will be input.

```
Skip Begin options
Scale all variables
End options

Begin options 2
Scale linear variables
End options 2
```

The keyword Endrun prevents subroutine dnSpec from reading past that point in the Specs file while looking for Begin.

4.3. SPECS file checklist and defaults

The following example Specs file shows all valid *keywords* and their *default values*. The keywords are grouped according to the function they perform.

Some of the default values depend on ϵ , the relative precision of the machine being used. The values given here correspond to double-precision arithmetic on most current machines ($\epsilon \approx 2.22 \times 10^{-16}$).

```
BEGIN checklist of SPECS file parameters and their default values
* Printing
  Major print level
                                   1
                                            * 1-line major iteration log
  Minor print level
                                   1
                                            * 1-line minor iteration log
                                            * specified by subroutine dnBEGIN
  Print
          file
                                   ?
                                            * specified by subroutine dnBEGIN
  Summary file
                                 100
  Print frequency
                                            * minor iterations log on Print file
                                 100
  Summary frequency
                                            * minor iterations log on Summary file
                                            * on the Print file
  Solution
                                 Yes
* Suppress options listing
                                            * options are normally listed
  System information
                                  No
                                            * Yes prints more system information
* Problem specification
  Minimize
                                            * (opposite of Maximize)
* Feasible point
                                              (alternative to Max or Min)
  Infinite bound
                                   1.0e+20 *
* Convergence Tolerances
  Major feasibility tolerance
                                   1.0e-6 * target nonlinear constraint violation
  Major optimality tolerance
                                   1.0e-6 * target complementarity gap
  Minor feasibility tolerance
                                   1.0e-6 * for satisfying the QP bounds
* Derivative checking
  Verify level
                                   Λ
                                            * cheap check on gradients
  Start objective check at col 1
  Stop objective check at col n_1'
  Start constraint check at col 1
  Stop constraint check at col n_1''
* Scaling
  Scale option
                                   1
                                            * linear constraints and variables
  Scale tolerance
                                   0.9
* Scale Print
                                            * default: scales are not printed
* Other Tolerances
  Crash tolerance
                                   0.1
                                   0.9
                                            * smaller for more accurate search
  Linesearch tolerance
                                   3.7e-11 * \epsilon^{2/3}
  Pivot tolerance
* QP subproblems
                                   1.0e+4 * used only during elastic mode
  Elastic weight
  Iterations limit
                                   10000
                                            * or 20m if that is more
  Partial price
                                            * 10 for large LPs
* SQP method
* Cold start
                                            * has precedence over argument start
* Warm start
                                            * (alternative to a cold start)
```

```
Major iterations limit
                              1000
                                         * or m if that is more
 Minor iterations limit
                               500
                                         * or 3m if that is more
 Major step limit
                               2.0
 Superbasics limit
                                n_1 + 1 * n_1 = number of nonlinear variables
 Derivative level
                                 3
 Derivative linesearch
* Nonderivative linesearch
                                3.0e-13 * \epsilon^{0.8} (almost full accuracy)
 Function precision
 Difference interval 5.5e-7 * (Function precision)^{1/2}
 Central difference interval 6.7e-5 * (Function precision)^{1/3}
                                         * initial penalty parameter
 Penalty parameter
                                0.0
                              1
 Proximal point method
                                         * satisfies linear constraints near x_0
                                      * unscaled constraint violation limit
 Violation limit
                                10.0
 Unbounded step size
                                1.0e+18 *
 Unbounded objective
                                 1.0e+15 *
* Hessian approximation
 Hessian frequency
                            999999
                                         * for full Hessian (never reset)
 Hessian flush
                            999999
                                         * no flushing
* Frequencies
                                         * test row residuals ||Ax - s||
  Check frequency
                                60
 Expand frequency
                             10000
                                         * for anti-cycling procedure
                                         * 100 for LPs
 Factorization frequency
* Partitions of cw, iw, rw
 Total character workspace
                                 lencw
 Total integer workspace
                                 leniw
 Total real
                 workspace
                                 lenrw
                                 500
 User character workspace
                                 500
 User integer workspace
                  workspace
                                 500
 User real
* Miscellaneous
 Debug level
                                 0
                                         * for developers
 Sticky parameters
                                No
                                         * Yes makes parameter values persist
End of SPECS file checklist
```

4.4. Subroutine dnSpec

Subroutine dnSpec may be called to input a Specs file (to specify options for a subsequent call of DNOPT).

```
subroutine dnSpec

( iSpecs, INFO, cw, lencw, iw, leniw, rw, lenrw )
integer

iSpecs, INFO, lencw, leniw, lenrw, iw(leniw)
double precision

rw(lenrw)
character

cw(lencw)*8
```

On entry:

iSpecs is a unit number for the Specs file (iSpecs > 0). Typically iSpecs = 4.

On some systems, the file may need to be opened before dnSpec is called.

On exit:

cw(lencw), iw(leniw), rw(lenrw) contain the specified options.

INFO reports the result of calling dnSpec. Here is a summary of possible values.

Finished successfully

101 Specs file read.

 $Errors\ while\ reading\ Specs\ file$

- No Specs file specified (iSpecs ≤ 0 or iSpecs > 99).
- 132 End-of-file encountered while looking for Specs file. dnSpec encountered end-of-file or Endrun before finding Begin (see Section 4.2). The Specs file may not be properly assigned.
- End-of-file encountered before finding End. Lines containing Skip or Endrun may imply that all options should be ignored.
- 134 Endrun found before any valid sets of options.
- > 134 There were i = INFO 134 errors while reading the Specs file.

4.5. Subroutines dnSet, dnSetInt, dnSetReal

These routines specify an option that might otherwise be defined in one line of a Specs file.

```
subroutine dnSet
     &
          (buffer,
                             iPrint, iSumm, Errors,
                             cw, lencw, iw, leniw, rw, lenrw)
      subroutine dnSetInt
     &
          ( buffer, ivalue, iPrint, iSumm, Errors,
                             cw, lencw, iw, leniw, rw, lenrw)
      subroutine dnSetReal
         (buffer, rvalue, iPrint, iSumm, Errors,
     &
                             cw, lencw, iw, leniw, rw, lenrw)
      character*(*)
           buffer
      integer
           Errors, ivalue, iPrint, iSumm, lencw, leniw, lenrw, iw(leniw)
      double precision
           rvalue, rw(lenrw)
      character
           cw(lencw)*8
On entry:
buffer is a string to be decoded. Restriction: len(buffer) \leq 72 (dnSet) or \leq 55
       (dnSetInt, dnSetReal). Use dnSet if the string contains all relevant data. For
       example.
          call dnSet ('Iterations 1000',
                                                iPrint, iSumm, Errors, ...)
ivalue is an integer value associated with the keyword in buffer. Use dnSetInt if it is
       convenient to define the value at run time. For example,
          itnlim = 1000
          if (m.gt. 500) itnlim = 8000
          call dnSetInt( 'Iterations', itnlim, iPrint, iSumm, Errors, ... )
rvalue is a real value associated with the keyword in buffer. For example,
          factol = 100.0d+0
          if (illcon) factol = 5.0d+0
          call dnSetReal( 'LU factor tol', factol, iPrint, iSumm, Errors, ...)
iPrint is a file number for printing each line of data, along with any error messages. iPrint
       = 0 suppresses this output.
iSumm is a file number for printing any error messages. iSumm = 0 suppresses this output.
Errors is the cumulative number of errors, so it should be 0 before the first call in a group
       of calls to the option-setting routines.
```

On exit:

cw(lencw), iw(leniw), rw(lenrw) hold the specified option.

Errors is the number of errors encountered so far.

4.6. Subroutines dnGet, dnGetChar, dnGetInt, dnGetReal

These routines obtain the current value of a single option or indicate if an option has been set.

```
integer function dnGet
                              Errors, cw, lencw, iw, leniw, rw, lenrw )
          (buffer,
      subroutine dnGetChar
          ( buffer, cvalue, Errors, cw, lencw, iw, leniw, rw, lenrw )
      subroutine dnGetInt
          ( buffer, ivalue, Errors, cw, lencw, iw, leniw, rw, lenrw )
      subroutine dnGetReal
          ( buffer, rvalue, Errors, cw, lencw, iw, leniw, rw, lenrw )
      character*(*)
            buffer
      integer
            Errors, ivalue, lencw, leniw, lenrw, iw(leniw)
            cvalue*8, cw(lencw)*8
      double precision
            rvalue, rw(lenrw)
On entry:
buffer is a string to be decoded. Restriction: len(buffer) \leq 72.
Errors is the cumulative number of errors, so it should be 0 before the first call in a group
       of calls to option-getting routines.
cw(lencw), iw(leniw), rw(lenrw) contain the current options data.
On exit:
       is 1 if the option contained in buffer has been set, otherwise 0. Use dnGet to find if
       a particular optional parameter has been set. For example: if
           i = dnGet( 'Hessian limited memory', Errors, ... )
       then i will be 1 if DNOPT is using a limited-memory approximate Hessian.
cvalue is a string associated with the keyword in buffer. Use dnGetChar to obtain the
       names associated with an MPS file. For example, for the name of the bounds section
       use
```

call dnGetChar('Bounds', MyBounds, Errors, ...)

call dnGetInt('Iterations limit', itnlim, Errors, ...)

call dnGetReal('LU factor tol', factol, Errors, ...)

ivalue is an integer value associated with the keyword in buffer. Example:

rvalue is a real value associated with the keyword in buffer. Example:

Errors is the number of errors encountered so far.

4.7. Description of the optional parameters

The following is an alphabetical list of the options that may appear in the Specs file, and a description of their effect. In the description of the options we use the notation of the problem format NP to refer to the objective and constraint functions.

Central difference interval

 $\mathrm{Default} = \epsilon^{1/3} pprox$ 6.0e-6

When Derivative level < 3) with dnOpt, the central-difference interval r is used near an optimal solution to obtain more accurate (but more expensive) estimates of gradients. Twice as many function evaluations are required compared to forward differencing. The interval used for the jth variable is $h_j = r(1 + |x_j|)$. The resulting derivative estimates should be accurate to $O(r^2)$, unless the functions are badly scaled.

Check frequency

k

Default = 60

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

Check frequency 1 is useful for debugging purposes, but otherwise this option should not be needed.

Cold Start

Default = value of input argument start

Requests that the CRASH procedure be used to choose an initial working set.

This parameter has the same effect as the input arguments start = 0 for dnOpt. If specified as an optional parameter, this value has precedence over the value of the input argument start. This allows the start parameter to be changed at run-time using the Specs file.

Crash tolerance t Default = 0.1

This value is used in conjunction with the optional parameter Cold start (the default value). When making a cold start, the QP algorithm in dn0pt must select an initial working set. When $r \geq 0$, 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.

Derivative level i Default = 3

The keyword Derivative level specifies which nonlinear function gradients are known analytically and will be supplied to DNOPT by the user subroutines funobj and funcon.

- i Meaning
- 3 All objective and constraint gradients are known.
- 2 All constraint gradients are known, but some or all components of the objective gradient are unknown.

- 1 The objective gradient is known, but some or all of the constraint gradients are unknown.
- O Some components of the objective gradient are unknown and some of the constraint gradients are unknown.

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

If i = 0 or 2, DNOPT will estimate the missing components of the objective gradient, using finite differences. This may simplify the coding of subroutine funobj. However, it could increase the total run-time substantially (since a special call to funobj is required for each missing element), and there is less assurance that an acceptable solution will be located. If the nonlinear variables are not well scaled, it may be necessary to specify a nonstandard Difference interval (see below).

If i = 0 or 1, DNOPT will estimate missing elements of the Jacobian. For each column of the Jacobian, one call to funcon is needed to estimate all missing elements in that column, if any. If the Jacobian happens to be

where * indicates a known gradient and ? indicates an unknown element, DNOPT will use one call to funcon to estimate the missing element in column 2, and another call to estimate both missing elements in column 3. No calls are needed to estimate the elements in columns 1 and 4.

At times, central differences are used rather than forward differences. Twice as many calls to funobj and funcon are then needed. (This is not under the user's control.)

Derivative linesearch Nonderivative linesearch

Default

At each major iteration a linesearch is used to improve the merit function. A Derivative linesearch uses safeguarded cubic interpolation and requires both function and gradient values to compute estimates of the step α_k . If some analytic derivatives are not provided, or a Nonderivative linesearch is specified, DNOPT employs a linesearch based upon safeguarded quadratic interpolation, which does not require gradient evaluations.

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

The selection of Nonderivative linesearch for dnOpt means that funobj and funcon are called with mode = 0 in the linesearch. Once the linesearch is completed, the problem functions are called again with mode = 2. If the potential savings provided by a nonderivative linesearch are to be realized, it is essential that funobj and funcon be coded so that the derivatives are not computed when mode = 0.

Difference interval

 h_1

 $Default = \epsilon^{1/2} pprox$ 1.5e-8

This alters the interval h_1 that is used to estimate gradients by forward differences in the following circumstances:

- In the initial ("cheap") phase of verifying the problem derivatives.
- For verifying the problem derivatives.
- For estimating missing derivatives.

In all cases, a derivative with respect to x_j is estimated by perturbing that component of x to the value $x_j + h_1(1 + |x_j|)$, and then evaluating $f_0(x)$ or f(x) at the perturbed point. The resulting gradient estimates should be accurate to $O(h_1)$ unless the functions are badly scaled. Judicious alteration of h_1 may sometimes lead to greater accuracy.

Elastic weight ω Default = 10^4

This keyword determines the initial weight γ associated with problem NP(γ) on p. 10.

At major iteration k, if elastic mode has not yet started, a scale factor $\sigma_k = 1 + \|g(x_k)\|_{\infty}$ is defined from the current objective gradient. Elastic mode is then started if the QP subproblem is infeasible, or the QP dual variables are larger in magnitude than $\sigma_k \omega$. The QP is re-solved in elastic mode with $\gamma = \sigma_k \omega$.

Thereafter, major iterations continue in elastic mode until they converge to a point that is optimal for problem NP(γ). If the point is feasible for NP (v=w=0), it is declared locally optimal. Otherwise, γ is increased by a factor of 10 and major iterations continue. If γ has already reached a maximum allowable value, NP is declared locally infeasible.

Expand frequency k Default = 10000

This option is part of the EXPAND anti-cycling procedure [13] designed to make progress even on highly degenerate problems.

For linear models, the strategy is to force a positive step at every iteration, at the expense of violating the bounds on the variables by a small amount. Suppose that the Minor feasibility tolerance is δ . Over a period of k iterations, the tolerance actually used by DNOPT increases from $\frac{1}{2}\delta$ to δ (in steps of $\frac{1}{2}\delta/k$).

For nonlinear models, the same procedure is used for iterations in which there is only one superbasic variable. (Cycling can occur only when the current solution is at a vertex of the feasible region.) Thus, zero steps are allowed if there is more than one superbasic variable, but otherwise positive steps are enforced.

Increasing k helps reduce the number of slightly infeasible nonbasic variables (most of which are eliminated during a resetting procedure). However, it also diminishes the freedom to choose a large pivot element (see Pivot tolerance).

Factorization frequency k Default = 100 (LP) or 50 (NP)

At most k constraint changes will occur between factorizations of the working set matrix.

- With linear programs, the working-set factors are usually updated every iteration. The default k is reasonable for typical problems. Higher values up to k = 100 (say) may be more efficient on problems that are extremely sparse and well scaled.
- When the objective function is nonlinear, fewer updates to the working set will occur as an optimum is approached. The number of iterations between working set factorizations will therefore increase. During these iterations a test is made regularly (according to the Check frequency) to ensure that the general constraints are satisfied. If necessary the working set will be refactorized before the limit of k updates is reached.

Feasible point see Minimize

Function precision

 ϵ_R

 $\mathrm{Default} = \epsilon^{0.8} \approx \texttt{3.7e-11}$

The relative function precision ϵ_R is intended to be a measure of the relative accuracy with which the nonlinear functions can be computed. For example, if f(x) is computed as 1000.56789 for some relevant x and if the first 6 significant digits are known to be correct, the appropriate value for ϵ_R would be 1.0e-6.

(Ideally the functions f(x) or $F_i(x)$ should have magnitude of order 1. If all functions are substantially less than 1 in magnitude, ϵ_R should be the absolute precision. For example, if f(x) = 1.23456789e-4 at some point and if the first 6 significant digits are known to be correct, the appropriate value for ϵ_R would be 1.0e-10.)

- The default value of ϵ_R is appropriate for simple analytic functions.
- In some cases the function values will be the result of extensive computation, possibly involving an iterative procedure that can provide rather few digits of precision at reasonable cost. Specifying an appropriate Function precision may lead to savings, by allowing the linesearch procedure to terminate when the difference between function values along the search direction becomes as small as the absolute error in the values.

Feasibility tolerance see Minor feasibility tolerance

Default = 1.0e-6

Hessian frequency

i

t

Default = 999999

If Hessian Full is selected and *i* BFGS updates have already been carried out, the Hessian approximation is reset to the identity matrix. (For certain problems, occasional resets may improve convergence, but in general they should not be necessary.)

Hessian Full memory and Hessian frequency = 10 have a similar effect to Hessian Limited memory and Hessian updates = 10 (except that the latter retains the current diagonal during resets).

Infinite bound r Default = 1.0e+20

If r > 0, r 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 plus infinity (and similarly for a lower bound less than or equal to -infBnd). If $r \le 0$, the default value is used.

Iterations limit i Default = $\max\{10000, 20m\}$

This is the maximum number of minor iterations allowed (i.e., iterations of the simplex method or the QP algorithm), summed over all major iterations. (Itns is an alternative keyword.)

Linesearch tolerance t Default = 0.9

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

merit function is identified. This parameter determines the accuracy to which this target value is approximated.

- t must be a real value in the range $0.0 \le t \le 1.0$.
- The default value t = 0.9 requests just moderate accuracy in the linesearch.
- If the nonlinear functions are cheap to evaluate, a more accurate search may be appropriate; try t = 0.1, 0.01 or 0.001. The number of major iterations might decrease.
- If the nonlinear functions are expensive to evaluate, a less accurate search may be appropriate. If all gradients are known, try t=0.99. (The number of major iterations might increase, but the total number of function evaluations may decrease enough to compensate.)
- If not all gradients are known, a moderately accurate search remains appropriate. Each search will require only 1–5 function values (typically), but many function calls will then be needed to estimate missing gradients for the next iteration.

Log frequency see Print frequency

k

Default = 100

Major feasibility tolerance

 ϵ_r

Default = 1.0e-6

This specifies how accurately the nonlinear constraints should be satisfied. The default value of 1.0e-6 is appropriate when the linear and nonlinear constraints contain data to about that accuracy.

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

$$rowerr = \max_{i} \ viol_i / ||x|| \le \epsilon_r, \tag{4.1}$$

where $viol_i$ is the violation of the *i*th nonlinear constraint (i = 1 : nnCon).

In the major iteration log, rowerr appears as the quantity labeled "Feasibl". If some of the problem functions are known to be of low accuracy, a larger Major feasibility tolerance may be appropriate.

Major iterations limit

k

 $Default = \max\{1000, m\}$

This is the maximum number of major iterations allowed. It is intended to guard against an excessive number of linearizations of the constraints. If k = 0, both feasibility and optimality are checked.

Major optimality tolerance ϵ_d

Default = 1.0e-6

This specifies the final accuracy of the dual variables. On successful termination, DNOPT will have computed a solution (x, s, π) such that

$$\max \mathtt{Comp} = \max_{j} \ \mathtt{Comp}_{j} / \|\pi\| \ \leq \ \epsilon_{d}, \tag{4.2}$$

where $Comp_j$ is an estimate of the complementarity slackness for variable j (j = 1: n + m). The values $Comp_j$ are computed from the final QP solution using the reduced gradients

 $d_j = g_j - \pi^T a_j$ (where g_j is the jth component of the objective gradient, a_j is the associated column of the constraint matrix $\begin{pmatrix} A & -I \end{pmatrix}$, and π is the set of QP dual variables):

$$\mathtt{Comp}_j = \left\{ \begin{array}{ll} d_j \min\{x_j - l_j, 1\} & \quad \text{if } d_j \geq 0; \\ -d_j \min\{u_j - x_j, 1\} & \quad \text{if } d_j < 0. \end{array} \right.$$

In the major iteration log, maxComp appears as the quantity labeled "Optimal".

Major print level

p

Default = 00001

This controls the amount of output to the Print and Summary files each major iteration. Major print level 1 gives normal output for linear and nonlinear problems, and Major print level 11 gives addition details of the Jacobian factorization that commences each major iteration.

In general, the value being specified may be thought of as a binary number of the form

Major print level JFDXs

where each letter stands for a digit that is either 0 or 1 as follows:

- s a single line that gives a summary of each major iteration. (This entry in JFDXbs is not strictly binary since the summary line is printed whenever JFDXbs ≥ 1).
- $X x_k$, the nonlinear variables involved in the objective function or the constraints.
- D π_k , the dual variables for the nonlinear constraints.
- F $F(x_k)$, the values of the nonlinear constraint functions.
- J $J(x_k)$, the Jacobian matrix.

To obtain output of any items JFDXbs, set the corresponding digit to 1, otherwise to 0.

If J=1, the Jacobian matrix will be output column-wise at the start of each major iteration. Column j will be preceded by the value of the corresponding variable x_j and a key to indicate whether the variable is basic, superbasic or nonbasic. (Hence if J=1, there is no reason to specify X=1 unless the objective contains more nonlinear variables than the Jacobian.) A typical line of output is

3 1.250000D+01 BS

1 1.00000E+00

2.00000E+00

which would mean that x_3 is basic at value 12.5, and the third column of the Jacobian has elements of 1.0 and 2.0 in rows 1 and 4.

Major print level 0 suppresses most output, except for error messages.

Major step limit

r

Default = 2.0

This parameter limits the change in x during a linesearch. It applies to all nonlinear problems, once a "feasible solution" or "feasible subproblem" has been found.

- 1. A linesearch determines a step α over the range $0 < \alpha \le \beta$, where β is 1 if there are nonlinear constraints, or the step to the nearest upper or lower bound on x if all the constraints are linear. Normally, the first steplength tried is $\alpha_1 = \min(1, \beta)$.
- 2. In some cases, such as $f(x) = ae^{bx}$ or $f(x) = ax^b$, even a moderate change in the components of x can lead to floating-point overflow. The parameter r is therefore used to define a limit $\bar{\beta} = r(1 + ||x||)/||p||$ (where p is the search direction), and the first evaluation of f(x) is at the potentially smaller steplength $\alpha_1 = \min(1, \bar{\beta}, \beta)$.

- 3. Wherever possible, upper and lower bounds on x should be used to prevent evaluation of nonlinear functions at meaningless points. The Major step limit provides an additional safeguard. The default value r=2.0 should not affect progress on well behaved problems, but setting r=0.1 or 0.01 may be helpful when rapidly varying functions are present. A "good" starting point may be required. An important application is to the class of nonlinear least-squares problems.
- 4. In cases where several local optima exist, specifying a small value for r may help locate an optimum near the starting point.

Minimize Default

Maximize

Feasible point

The keywords Minimize and Maximize specify the required direction of optimization. It applies to both linear and nonlinear terms in the objective.

The keyword feasible point means "Ignore the objective function" while finding a feasible point for the linear and nonlinear constraints. It can be used to check that the nonlinear constraints are feasible without altering the call to DNOPT.

Minor iterations limit k Default = 500

If the number of minor iterations for the optimality phase of the QP subproblem exceeds k, then all nonbasic QP variables that have not yet moved are frozen at their current values and the reduced QP is solved to optimality.

Note that more than k minor iterations may be necessary to solve the reduced QP to optimality. These extra iterations are necessary to ensure that the terminated point gives a suitable direction for the linesearch.

In the major iteration log, a t at the end of a line indicates that the corresponding QP was artificially terminated using the limit k.

Note that Iterations limit defines an independent *absolute* limit on the *total* number of minor iterations (summed over all QP subproblems).

Minor feasibility tolerance t Default = 1.0e-6

DNOPT tries to ensure that all variables eventually satisfy their upper and lower bounds to within the tolerance t. This includes slack variables. Hence, general linear constraints should also be satisfied to within t.

Feasibility with respect to nonlinear constraints is judged by the Major feasibility tolerance (not by t).

- If the bounds and linear constraints cannot be satisfied to within t, the problem is declared *infeasible*. Let sInf be the corresponding sum of infeasibilities. If sInf is quite small, it may be appropriate to raise t by a factor of 10 or 100. Otherwise, some error in the data should be suspected.
- Nonlinear functions will be evaluated only at points that satisfy the bounds and linear
 constraints. If there are regions where a function is undefined, every attempt should
 be made to eliminate these regions from the problem.

For example, if $f(x) = \sqrt{x_1} + \log x_2$, it is essential to place lower bounds on both variables. If t = 1.0e-6, the bounds $x_1 \ge 10^{-5}$ and $x_2 \ge 10^{-4}$ might be appropriate. (The log singularity is more serious. In general, keep x as far away from singularities as possible.)

- If Scale option ≥ 1 , feasibility is defined in terms of the *scaled* problem (since it is then more likely to be meaningful).
- In reality, DNOPT uses t as a feasibility tolerance for satisfying the bounds on x and s in each QP subproblem. If the sum of infeasibilities cannot be reduced to zero, the QP subproblem is declared infeasible. DNOPT is then in *elastic mode* thereafter (with only the linearized nonlinear constraints defined to be elastic). See the Elastic options.

Minor print level

k

Default = 1

This controls the amount of output to the Print and Summary files during solution of the QP subproblems. The value of k has the following effect:

- 0 No minor iteration output except error messages.
- ≥ 1 A single line of output each minor iteration (controlled by Print frequency and Summary frequency).
- ≥ 10 Factorization statistics generated during the periodic refactorization of the working set (see Factorization frequency). Statistics for the *first factorization* each major iteration are controlled by the Major print level.

Pivot tolerance

t

Default = $\epsilon^{2/3} \approx 3.7e-11$

During solution of QP subproblems, the pivot tolerance is used to prevent constraints from entering the working set if they would cause the working set to become almost singular.

- When x changes to $x + \alpha p$ for some search direction p, a "ratio test" determines which component of x reaches an upper or lower bound first. The corresponding element of p is called the *pivot element*.
- Elements of p are ignored (and therefore cannot be pivot elements) if they are smaller than the pivot tolerance t.
- It is common for two or more variables to reach a bound at essentially the same time. In such cases, the Feasibility tolerance provides some freedom to maximize the pivot element and thereby improve numerical stability. An excessively small Feasibility tolerance should therefore not be specified.
- To a lesser extent, the Expand frequency also provides some freedom to maximize the pivot element. Hence, an excessively large Expand frequency should not be specified.

Print file
Print frequency

f 1

Default = 100

If f > 0, the Print file is output to file number f. If Minor print level > 0, a line of the QP iteration log is output every kth iteration. The default f is obtained from subroutine dnBEGIN's parameter iPrint. Set f = 0 to suppress output to the Print file.

Proximal point method

i

Default = 1

i = 1 or 2 specifies minimization of $||x - x_0||_1$ or $\frac{1}{2}||x - x_0||_2^2$ when the starting point x_0 is changed to satisfy the linear constraints (where x_0 refers to nonlinear variables).

Scale option $i \qquad \qquad \text{Default} = 2 \; \text{(LP) or 1 (NP)} \\ \text{Scale tolerance} \qquad \qquad t \qquad \qquad \text{Default} = 0.9 \\ \text{Scale Print}$

Three scale options are available as follows:

- i Meaning
- 0 No scaling. This is recommended if it is known that x and the constraint matrix (and Jacobian) never have very large elements (say, larger than 100).
- 1 Linear constraints and variables are scaled by an iterative procedure that attempts to make the matrix coefficients as close as possible to 1.0 (see Fourer [6]). This will sometimes improve the performance of the solution procedures.
- All constraints and variables are scaled by the iterative procedure. Also, an additional scaling is performed that takes into account columns of $\begin{pmatrix} A & -I \end{pmatrix}$ that are fixed or have positive lower bounds or negative upper bounds.

If nonlinear constraints are present, the scales depend on the Jacobian at the first point that satisfies the linear constraints. Scale option 2 should therefore be used only if (a) a good starting point is provided, and (b) the problem is not highly nonlinear.

Scale tolerance t affects how many passes might be needed through the constraint matrix. On each pass, the scaling procedure computes the ratio of the largest and smallest nonzero coefficients in each column:

$$\rho_j = \max_i |a_{ij}| / \min_i |a_{ij}| \qquad (a_{ij} \neq 0).$$

If $\max_j \rho_j$ is less than t times its previous value, another scaling pass is performed to adjust the row and column scales. Raising t from 0.9 to 0.99 (say) usually increases the number of scaling passes through A. At most 10 passes are made.

Scale Print causes the row-scales r(i) and column-scales c(j) to be printed. The scaled matrix coefficients are $\bar{a}_{ij} = a_{ij}c(j)/r(i)$, and the scaled bounds on the variables and slacks are $\bar{l}_j = l_j/c(j)$, $\bar{u}_j = u_j/c(j)$, where $c(j) \equiv r(j-n)$ if j > n.

Default = 0

The first three options determine whether the final solution obtained is to be output to the Print file. The file option operates independently; if f > 0, the final solution will be output to file f (whether optimal or not).

- For the Yes and If Optimal options, floating-point numbers are printed in f16.5 format, and "infinite" bounds are denoted by the word None.
- For the file option, all numbers are printed in 1p,e16.6 format, including "infinite" bounds, which will have magnitude infBnd (default value 1.000000e+20).

• To see more significant digits in the printed solution, it is sometimes useful to make f refer to the Print file (i.e., the number specified by Print file).

Start	Objective	Check	at	Column	k	Default = 1
Start	${\tt Constraint}$	Check	at	Column	k	Default = 1
Stop	Objective	Check	at	Column	l	$Default = n_1'$
Stop	${\tt Constraint}$	Check	at	Column	l	Default = n_1''

The default values depend on n'_1 and n''_1 , the numbers of nonlinear objective variables and Jacobian variables (see p. 13).

If Verify level > 0, these options may be used to abbreviate the verification of individual derivative elements computed by subroutines funobj, funcon and usrfun. For example:

- If the first 100 objective gradients appeared to be correct in an earlier run, and if you have just found a bug in funobj that ought to fix up the 101-th component, then you might as well specify Start Objective Check at Column 101. Similarly for columns of the Jacobian.
- If the first 100 variables occur nonlinearly in the constraints, and the remaining variables are nonlinear only in the objective, then funobj must set the first 100 components of g(*) to zero, but these hardly need to be verified. The above option would again be appropriate.

Sticky parameters No Default Sticky parameters Yes

User-defined optional parameters may be modified so that they lie in a sensible range. For example, any tolerance specified as negative or zero will be changed to its positive default value. Specifying Sticky parameters No will result in the original user-defined parameters being reloaded into workspace after the run is completed. If a second run is made immediatly following a call with Sticky parameters Yes (e.g., with the Hot start option) then any modified parameter values will persist in workspace for the second run.

Summary file f Summary frequency k Default = 100

If f > 0, the Summary file is output to file f. If Minor print level > 0, a line of the QP iteration log is output every kth minor iteration. The default f is obtained from subroutine dnBEGIN's parameter iSumm. Set f = 0 to suppress the Summary file.

Superbasics limit i Default $= n_1 + 1$

This places a limit on the storage allocated for superbasic variables. Ideally, i should be set slightly larger than the "number of degrees of freedom" expected at an optimal solution.

For linear programs, an optimum is normally a basic solution with no degrees of freedom. (The number of variables lying strictly between their bounds is no more than m, the number of general constraints.) The default value of i is therefore 1.

For nonlinear problems, the number of degrees of freedom is often called the "number of independent variables".

Normally, i need not be greater than n_1+1 , where n_1 is the number of nonlinear variables. For many problems, i may be considerably smaller than n_1 . This will save storage if n_1 is very large.

Suppress parameters

Normally DNOPT prints the Specs file as it is being read, and then prints a complete list of the available keywords and their final values. The Suppress Parameters option tells DNOPT not to print the full list.

Total	real	workspace	maxrw	Default = lenrw
Total	integer	workspace	maxiw	$Default = \mathtt{leniw}$
Total	character	workspace	maxcw	Default = lencw
User	real	workspace	maxru	Default = 500
User	integer	workspace	maxiu	Default = 500
User	character	workspace	maxcu	Default = 500

These options may be used to confine DNOPT to certain parts of its workspace arrays cw, iw, rw. (The arrays are defined by the last six parameters of DNOPT.)

The Total ... options place an *upper* limit on DNOPT's workspace. They may be useful on machines with virtual memory. For example, some systems allow a very large array rw(lenrw) to be declared at compile time with no overhead in saving the resulting object code. At run time, when various problems of different size are to be solved, it may be sensible to restrict DNOPT to the lower end of rw in order to reduce paging activity slightly. (However, DNOPT accesses storage contiguously wherever possible, so the benefit may be slight. In general it is far better to have too much storage than not enough.)

If DNOPT's "user" parameters ru, lenru happen to be the same as rw, lenrw, the nonlinear function routines will be free to use ru(maxrw + 1:lenru) for their own purpose. Similarly for the other work arrays.

The User ... options place a *lower* limit on DNOPT's workspace (not counting the first 500 elements). Again, if DNOPT's parameters ru, lenru happen to be the same as rw, lenrw, the function routines will be free to use ru(501:maxru) for their own purpose. Similarly for the other work arrays.

System information No Default System information Yes

The Yes option provides additional information on the progress of the iterations.

Timing level ℓ Default = 3

 $\ell = 0$ suppresses output of cpu times. (Intended for installations with dysfunctional timing routines.)

Unbounded objective value $f_{
m max}$ Default = 1.0e+15 Unbounded step size $\alpha_{
m max}$ Default = 1.0e+18

These parameters are intended to detect unboundedness in nonlinear problems. (They may not achieve that purpose!) During a linesearch, f_0 is evaluated at points of the form $x + \alpha p$, where x and p are fixed and α varies. if $|f_0|$ exceeds f_{\max} or α exceeds f_{\max} , iterations are terminated with the exit message Problem is unbounded (or badly scaled).

If singularities are present, unboundedness in $f_0(x)$ may be manifested by a floating-point overflow (during the evaluation of $f_0(x + \alpha p)$), before the test against f_{max} can be made.

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

Verify level l Default = 0

This option refers to finite-difference checks on the derivatives computed by the user-provided routines. Derivatives are checked at the first point that satisfies all bounds and linear constraints.

- l Meaning
- Only a "cheap" test will be performed, requiring 2 calls to funcon and 3 calls to funobj for dnOpt.
- 1 Individual objective gradients will be checked (with a more reliable test). A key of the form "OK" or "Bad?" indicates whether or not each component appears to be correct.
- 2 Individual columns of the problem Jacobian will be checked.
- 3 Options 2 and 1 will both occur (in that order).
- -1 Derivative checking is disabled.

Verify level 3 should be specified whenever a new function routine is being developed. The Start and Stop keywords may be used to limit the number of nonlinear variables checked. Missing derivatives are not checked, so they result in no overhead.

Violation limit au Default = 10

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

$$v_i(x_{k+1}) \le \tau \max\{1, v_i(x_0)\},\tag{4.3}$$

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

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

Warm start Default = value of input argument start

This parameter indicates that a working set is already specified via the input arrays for DNOPT. This option has the same effect as the input arguments start = 2. If specified as an optional parameter, this value has precedence over the value of the input argument start. This allows the start parameter to be changed at run-time using the Specs file.

Subroutine dnBEGIN specifies unit numbers for the Print and Summary files described in this section. The files can be redirected with the Print file and Summary file options (or suppressed).

5.1. The PRINT file

If Print file > 0, the following information is output to the Print file during the solution process. All printed lines are less than 131 characters.

- A listing of the Specs file, if any.
- A listing of the options that were or could have been set in the Specs file.
- An estimate of the working storage needed and the amount available.
- Some statistics about the problem being solved.
- A summary of the scaling procedure, if Scale option > 0.
- Notes about the initial working set resulting from a CRASH procedure.
- The major iteration log.
- The minor iteration log.
- The EXIT condition and some statistics about the solution obtained.
- The printed solution, if requested.

The last five items are described in the following sections.

5.2. The major iteration log

If Major print level > 0, one line of information is output to the Print file every kth minor iteration, where k is the specified Print frequency (default k = 1).

Label Description

Itns The cumulative number of minor iterations.

Major The current major iteration number.

Minors is the number of iterations required by both the feasibility and optimality phases of the QP subproblem. Generally, Minors will be 1 in the later iterations, since theoretical analysis predicts that the correct active set will be identified near the solution (see Section 2).

Step The step length α taken along the current search direction p. The variables x have just been changed to $x + \alpha p$. On reasonably well-behaved problems, the unit step will be taken as the solution is approached.

nCon The number of times subroutines usrfun or funcon have been called to evaluate the nonlinear problem functions. Evaluations needed for the estimation of the derivatives by finite differences are not included. nCon is printed as a guide to the amount of work required for the linesearch.

Feasible is the value of rowerr, the maximum component of the scaled nonlinear constraint residual (4.1). The solution is regarded as acceptably feasible if Feasible is less than the Major feasibility tolerance. In this case, the entry is contained in parenthesis.

If the constraints are linear, all iterates are feasible and this entry is not printed.

Optimal is the value of maxgap, the maximum complementarity gap (4.2). It is an estimate of the degree of nonoptimality of the reduced costs. Both Feasbl and Optimal are small in the neighborhood of a solution.

MeritFunction is the value of the augmented Lagrangian merit function (see (2.4)). This function will decrease at each iteration unless it was necessary to increase the penalty parameters (see Section 2). As the solution is approached, Merit will converge to the value of the objective at the solution.

In elastic mode, the merit function is a composite function involving the constraint violations weighted by the elastic weight.

If the constraints are linear, this item is labeled Objective, the value of the objective function. It will decrease monotonically to its optimal value.

nZ The current number of degrees of freedom.

CondHz An estimate of the condition number of R^TR , an estimate of Z^THZ , the reduced Hessian of the Lagrangian. It is the square of the ratio of the largest and smallest diagonals of the upper triangular matrix R (which is a lower bound on the condition number of R^TR). Cond Hz gives a rough indication of whether or not the optimization procedure is having difficulty. If ϵ is the relative precision of the machine being used, the SQP algorithm will make slow progress if Cond Hz becomes as large as $\epsilon^{-1/2} \approx 10^8$, and will probably fail to find a better solution if Cond Hz reaches $\epsilon^{-3/4} \approx 10^{12}$.

To guard against high values of Cond Hz, attention should be given to the scaling of the variables and the constraints. In some cases it may be necessary to add upper or lower bounds to certain variables to keep them a reasonable distance from singularities in the nonlinear functions or their derivatives.

Penalty is the Euclidean norm of the vector of penalty parameters used in the augmented Lagrangian merit function (not printed if there are no nonlinear constraints).

The summary line may include additional code characters that indicate what happened during the course of the major iteration.

Code Meaning

- c Central differences have been used to compute the unknown components of the objective and constraint gradients. A switch to central differences is made if either the linesearch gives a small step, or x is close to being optimal. In some cases, it may be necessary to re-solve the QP subproblem with the central-difference gradient and Jacobian.
- d During the linesearch it was necessary to decrease the step in order to obtain a maximum constraint violation conforming to the value of Violation limit.
- The norm-wise change in the variables was limited by the value of the Major step limit. If this output occurs repeatedly during later iterations, it may be worthwhile increasing the value of Major step limit.
- i If DNOPT is not in elastic mode, an "i" signifies that the QP subproblem is infeasible. This event triggers the start of nonlinear elastic mode, which remains in effect for all subsequent iterations. Once in elastic mode, the QP subproblems are associated with the elastic problem $NP(\gamma)$.

If DNOPT is already in elastic mode, an "i" indicates that the minimizer of the elastic subproblem does not satisfy the linearized constraints. (In this case, a feasible point for the usual QP subproblem may or may not exist.)

- M An extra evaluation of the problem functions was needed to define an acceptable positive-definite quasi-Newton update to the Lagrangian Hessian. This modification is only done when there are nonlinear constraints.
- m This is the same as "M" except that it was also necessary to modify the update to include an augmented Lagrangian term.
- n No positive-definite BFGS update could be found. The approximate Hessian is unchanged from the previous iteration.
- R The approximate Hessian has been reset by discarding all but the diagonal elements. This reset will be forced periodically by the Hessian frequency and Hessian updates keywords. However, it may also be necessary to reset an ill-conditioned Hessian from time to time.
- The approximate Hessian was reset after ten consecutive major iterations in which no BFGS update could be made. The diagonals of the approximate Hessian are retained if at least one update has been done since the last reset. Otherwise, the approximate Hessian is reset to the identity matrix.
- s A self-scaled BFGS update was performed. This update is used when the Hessian approximation is diagonal, and hence always follows a Hessian reset.
- t The minor iterations were terminated because of the Minor iterations limit.
- T The minor iterations were terminated because of the New superbasics limit.
- u The QP subproblem was unbounded.
- w A weak solution of the QP subproblem was found.
- z The Superbasics limit was reached.

5.3. The minor iteration log

If Minor print level > 0, one line of information is output to the Print file every kth minor iteration, where k is the specified Minor print frequency (default k = 1). A heading is printed before the first such line following a matrix factorization.

The heading contains the items described below.

Label Description

Itn The current iteration number.

Step The step length α taken along the current search direction p. The variables x have just been changed to $x + \alpha p$. If a constraint is added to the working set during the current iteration, Step will be the step to the nearest bound. During Phase 2, the step can be greater than one only if the reduced Hessian is not positive definite.

nInf The number of infeasibilities *after* the present iteration. This number will not increase unless the iterations are in elastic mode.

SumInf If nInf > 0, this is sInf, the sum of infeasibilities after the present iteration. It usually decreases at each nonzero Step, but if nInf decreases by 2 or more, SumInf may occasionally increase.

In elastic mode, the heading is changed to Composite Obj, and the value printed decreases monotonically.

gZnorm The norm of the reduced-gradient vector at the start of the iteration. During Phase 2 this norm will be approximately zero after a unit step.

(The heading is not printed if the problem is linear.)

QP objective, Elastic QPobj The QP objective function after the present iteration. In elastic mode, the heading is changed to Elastic QPobj. In either case, the value printed decreases monotonically.

+ymul The constraint index selected to be deleted from the working set.

nZ The current number of degrees of freedom. (The heading is not printed if the problem is linear.)

cond Hz See the major iteration log. (The heading is not printed if the problem is linear.)

5.4. EXIT conditions

When any solver or auxliliary routine in the DNOPT package terminates, a message of the following form is output to the Print and Summary files:

```
SOLVER EXIT \,e -- exit condition SOLVER INFO \,i -- informational message
```

where e is an integer that labels a generic exit condition, and i labels one of several alternative informational messages. For example, DNOPT may output

```
DNOPT EXIT 20 -- the problem appears to be unbounded DNOPT INFO 21 -- unbounded objective
```

where the exit condition gives a broad definition of what happened, while the informational message is more specific about the cause of the termination. The integer i is the value of the output argument INFO. The integer e may be recovered from INFO by changing the least significant digit to zero. Possible exit conditions for DNOPT follow:

- 0 Finished successfully
- 10 The problem appears to be infeasible
- 20 The problem appears to be unbounded
- 30 Resource limit error
- 40 Terminated after numerical difficulties
- 50 Error in the user-supplied functions
- 60 Undefined user-supplied functions
- 70 User requested termination
- 80 Insufficient storage allocated
- 90 Input arguments out of range
- 100 Finished successfully (associated with DNOPT auxiliary routines)
- 110 Errors while processing MPS data
- 120 Errors while estimating Jacobian structure
- 130 Errors while reading the Specs file
- 140 System error

Exit conditions 0–20 arise when a solution exists (though it may not be optimal). A basis file may be saved, and the solution is output to the Print or Solution files if requested.

If exit conditions 80–100 occur during the *first* basis factorization, the primal and dual variables **x** and **pi** will have their original input values. Basis files are saved if requested, but certain values in the printed solution will not be meaningful.

We describe each exit message from DNOPT and suggest possible courses of action.

DNOPT

```
EXIT --
            finished successfully
INFO --
            optimality conditions satisfied
            feasible point found
                                     (from option Feasible point only)
INFO --
            requested accuracy could not be achieved
```

These messages usually indicate a successful run. Basis files are saved, and the solution is printed and/or saved on the Solution file.

For INFO 1 the final point seems to be a solution of NP. This means that x is feasible (it satisfies the constraints to the accuracy requested by the Feasibility tolerance), the reduced gradient is negligible, the reduced costs are optimal, and R is nonsingular.

In all cases, some caution should be exercised. For example, if the objective value is much better than expected, DNOPT may have obtained an optimal solution to the wrong problem! Almost any item of data could have that effect if it has the wrong value. Verifying that the problem has been defined correctly is one of the more difficult tasks for a model builder. It is good practice in the function subroutines to print any data that is input during the first entry.

If nonlinearities exist, one must always ask the question: could there be more than one local optimum? When the constraints are linear and the objective is known to be convex (e.g., a sum of squares) then all will be well if we are minimizing the objective: a local minimum is a global minimum in the sense that no other point has a lower function value. (However, many points could have the same objective value, particularly if the objective is largely linear.) Conversely, if we are maximizing a convex function, a local maximum cannot be expected to be global, unless there are sufficient constraints to confine the feasible region.

Similar statements could be made about nonlinear constraints defining convex or concave regions. However, the functions of a problem are more likely to be neither convex nor concave. Our advice is always to specify a starting point that is as good an estimate as possible, and to include reasonable upper and lower bounds on all variables, in order to confine the solution to the specific region of interest. We expect modelers to know something about their problem, and to make use of that knowledge as they themselves know best.

One other caution about "Optimality conditions satisfied". Some of the variables or slacks may lie outside their bounds more than desired, especially if scaling was requested. Some information concerning the run can be obtained from the short summary given at the end of the print and summary files. Here is an example from the problem Toy discussed in Section 3.2.

```
0 -- finished successfully
DNOPT
                1 -- optimality conditions satisfied
Problem name
                              Toy
No. of iterations
                                         Objective value
                                                               1.9001249926E+00
                                    16
No. of major iterations
                                    13
                                         Linear objective
                                                               9.9624996883E-02
Penalty parameter
                             6.080E+00
                                         Nonlinear objective
                                                              1.8004999958E+00
No. of calls to funobj
                                    24
                                         No. of calls to funcon
                                                                             23
Degrees of freedom
                                     1
                                     0
No. of degenerate steps
                                         Percentage
                                                                           0.00
```

Max Primal infeas refers to the largest bound infeasibility and which variable is involved. If it is too large, consider restarting with a smaller Minor feasibility tolerance (say 10 times smaller) and perhaps Scale option 0.

Similarly, Max Dual infeas indicates which variable is most likely to be at a non-optimal value. Broadly speaking, if

```
Max Dual infeas/Max pi = 10^{-d},
```

then the objective function would probably change in the dth significant digit if optimization could be continued. If d seems too large, consider restarting with a smaller Major optimality tolerance.

Finally, Nonlinear constraint violn shows the maximum infeasibility for nonlinear rows. If it seems too large, consider restarting with a smaller Major feasibility tolerance.

If the requested accuracy could not be achieved, a feasible solution has been found, but the requested accuracy in the dual infeasibilities could not be achieved. An abnormal termination has occurred, but DNOPT is within 10^{-2} of satisfying the Major optimality tolerance. Check that the Major optimality tolerance is not too small.

```
EXIT -- 10 The problem appears to be infeasible
```

INFO -- 11 infeasible linear constraints

INFO -- 12 infeasible linear equalities

INFO -- 13 nonlinear infeasibilities minimized

INFO -- 14 infeasibilities minimized

This exit occurs if DNOPT is unable to find a point satisfying the constraints.

When the constraints are *linear*, the output messages are based on a relatively reliable indicator of infeasibility. Feasibility is measured with respect to the upper and lower bounds on the variables and slacks. Among all the points satisfying the general constraints Ax - s = 0, there is apparently no point that satisfies the bounds on x and s. Violations as small as the Minor feasibility tolerance are ignored, but at least one component of x or s violates a bound by more than the tolerance.

When nonlinear constraints are present, infeasibility is much harder to recognize correctly. Even if a feasible solution exists, the current linearization of the constraints may not contain a feasible point. In an attempt to deal with this situation, when solving each QP subproblem, DNOPT is prepared to relax the bounds on the slacks associated with nonlinear rows

If a QP subproblem proves to be infeasible or unbounded (or if the Lagrange multiplier estimates for the nonlinear constraints become large), DNOPT enters so-called "nonlinear elastic" mode. The subproblem includes the original QP objective and the sum of the infeasibilities—suitably weighted using the Elastic weight parameter. In elastic mode, some of the bounds on the nonlinear rows "elastic"—i.e., they are allowed to violate their specified bounds. Variables subject to elastic bounds are known as elastic variables. An elastic variable is free to violate one or both of its original upper or lower bounds. If the original problem has a feasible solution and the elastic weight is sufficiently large, a feasible point eventually will be obtained for the perturbed constraints, and optimization can continue on the subproblem. If the nonlinear problem has no feasible solution, DNOPT will tend to determine a "good" infeasible point if the elastic weight is sufficiently large. (If the elastic weight were infinite, DNOPT would locally minimize the nonlinear constraint violations subject to the linear constraints and bounds.)

Unfortunately, even though DNOPT locally minimizes the nonlinear constraint violations, there may still exist other regions in which the nonlinear constraints are satisfied. Wherever possible, nonlinear constraints should be defined in such a way that feasible points are known to exist when the constraints are linearized.

```
EXIT -- 20 The problem appears to be unbounded
```

INFO -- 21 unbounded objective

INFO -- 22 constraint violation limit reached

For linear problems, unboundedness is detected by the simplex method when a nonbasic variable can be increased or decreased by an arbitrary amount without causing a basic variable to violate a bound. A message prior to the EXIT message will give the index of the nonbasic variable. Consider adding an upper or lower bound to the variable. Also, examine the constraints that have nonzeros in the associated column, to see if they have been formulated as intended.

Very rarely, the scaling of the problem could be so poor that numerical error will give an erroneous indication of unboundedness. Consider using the Scale option.

For nonlinear problems, DNOPT monitors both the size of the current objective function and the size of the change in the variables at each step. If either of these is very large (as judged by the Unbounded parameters—see Section 4.7), the problem is terminated and declared unbounded. To avoid large function values, it may be necessary to impose bounds on some of the variables in order to keep them away from singularities in the nonlinear functions.

The second informational message indicates an abnormal termination while enforcing the limit on the constraint violations. This exit implies that the objective is not bounded below in the feasible region defined by expanding the bounds by the value of the Violation limit.

```
EXIT -- 30 Resource limit error

INFO -- 31 iteration limit reached

INFO -- 32 major iteration limit reached

INFO -- 33 the superbasics limit is too small
```

Some limit was exceeded before the required solution could be found. Check the iteration log to be sure that progress was being made. If so, restart the run using a basis file that was saved (or should have been saved!) at the end of the run.

If the superbasics limit is too small, then the problem appears to be more nonlinear than anticipated. The current set of basic and superbasic variables have been optimized as much as possible and a PRICE operation is necessary to continue, but there are already Superbasics limit superbasics (and no room for any more).

In general, raise the Superbasics limit s by a reasonable amount, bearing in mind the storage needed for the reduced Hessian. (The Reducd Hessian dimension h will also increase to s unless specified otherwise, and the associated storage will be about $\frac{1}{2}s^2$ words.) In some cases you may have to set h < s to conserve storage. The QPSolver CG option will be invoked and the rate of convergence will probably fall off severely.

```
EXIT -- 40 Terminated after numerical difficulties INFO -- 41 current point cannot be improved INFO -- 42 singular basis INFO -- 43 cannot satisfy the general constraints INFO -- 44 ill-conditioned null-space basis
```

These conditions arise only after the LU factorization options have been strengthened (automatically) as much as possible.

For INFO 41, DNOPT was unable to improve on a non-optimal point.

- 1. Subroutines usrfun, funobj or funcon may be returning accurate function values but inaccurate gradients (or vice versa). This is the most likely cause. Study the comments given for INFO 51 and 52, and check that the coding of the problem functions is correct.
- 2. The function and gradient values could be consistent, but their precision could be too low. For example, accidental use of a real data type when double precision was intended would lead to a relative function precision of about 10^{-6} instead of something like 10^{-15} . The default Major optimality tolerance of 10^{-6} would need to be raised

 $5. \quad Output$

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to about 10^{-3} for optimality to be declared (at a rather suboptimal point). Of course, it is better to revise the function coding to obtain as much precision as economically possible.

3. If function values are obtained from an expensive iterative process, they may be accurate to rather few significant figures, and gradients will probably not be available. One should specify

Function precision t Major optimality tolerance \sqrt{t}

but even then, if t is as large as 10^{-5} or 10^{-6} (only 5 or 6 significant figures), the same exit condition may occur. At present the only remedy is to increase the accuracy of the function calculation.

For INFO 42, the first factorization attempt found the basis to be structurally or numerically singular. (Some diagonals of the triangular matrix U were deemed too small.) The associated variables were replaced by slacks and the modified basis refactorized, but singularity persisted.

For INFO 43, the basic variables x_B have been recomputed, given the present values of the superbasic and nonbasic variables. A step of "iterative refinement" has also been applied to increase the accuracy of x_B , but a row check has revealed that the resulting solution does not satisfy the QP constraints Ax - s = b sufficiently well.

For INFO 44, during computation of the reduced Hessian Z^THZ , some column(s) of Z continued to contain very large values.

In all cases, the problem must be badly scaled (or the basis must be pathologically ill-conditioned without containing any large entries). Try Scale option 2 if it has not yet been used.

EXIT -- 50 Error in the user-supplied functions INFO -- 51 incorrect objective derivatives INFO -- 52 incorrect constraint derivatives

There may be errors in the subroutines that define the problem objective and constraints. If the objective derivatives appear to incorrect, a check has been made on some individual elements of the objective gradient array at the first point that satisfies the linear constraints. At least one component (G(k) or gObj(j)) is being set to a value that disagrees markedly with its associated forward-difference estimate $\partial f_0/\partial x_j$. (The relative difference between the computed and estimated values is 1.0 or more.) This exit is a safeguard because DNOPT will usually fail to make progress when the computed gradients are seriously inaccurate. In the process it may expend considerable effort before terminating with INFO 41 above.

For INFO 51 Check the function and gradient computation very carefully in usrfun or funobj. A simple omission (such as forgetting to divide f_0 by 2) could explain the discrepancy. If f_0 or a component $\partial f_0/\partial x_j$ is very large, then give serious thought to scaling the function or the nonlinear variables.

If you feel *certain* that the computed gObj(j) is correct (and that the forward-difference estimate is therefore wrong), you can specify Verify level 0 to prevent individual elements from being checked. However, the optimization procedure may have difficulty.

For INFO 52, at least one of the computed constraint derivatives is significantly different from an estimate obtained by forward-differencing the constraint vector f(x) of problem NP. Follow the advice for INFO 51, trying to ensure that the arrays F and G are being set correctly in usrfun or funcon.

```
EXIT -- 60 Undefined user-supplied functions
```

INFO -- 61 undefined function at the first feasible point

INFO -- 62 undefined function at the initial point

INFO -- 63 unable to proceed into undefined region

The parameter mode was assigned the value -1 in one of the user-defined routines usrfun, funobj or funcon. This value is used to indicate that the functions are undefined at the current point. DNOPT attempts to evaluate the problem functions closer to a point at which the functions have already been computed.

For INFO 61 and 62, DNOPT was unable to proceed because the functions are undefined at the initial point or the first feasible point.

For INFO 63, repeated attempts to move into a region where the functions are not defined resulted in the change in variables being unacceptably small. At the final point, it appears that the only way to decrease the merit function is to move into a region where the problem functions are not defined.

```
EXIT -- 70 User requested termination
```

INFO -- 71 terminated during function evaluation

INFO -- 72 terminated during constraint evaluation

INFO -- 73 terminated during objective evaluation

INFO -- 74 terminated from monitor routine

These exits occur when Status < -1 is set during some call to the user-defined routines. DNOPT assumes that you want the problem to be abandoned immediately.

```
EXIT -- 80 Insufficient storage allocated
```

INFO -- 81 work arrays must have at least 500 elements

INFO -- 82 not enough character storage

INFO -- 83 not enough integer storage

INFO -- 84 not enough real storage

DNOPT cannot start to solve a problem unless the character, integer, and real work arrays are at least 500 elements.

If the storage arrays cw(*), iw(*), rw(*) are not large enough for the current problem, an estimate of the additional storage required is given in messages preceding the exit. The routine declaring cw, iw, rw should be recompiled with larger dimensions lencw, leniw, lenrw.

If rw(*) is not large enough, be sure that the Reduced Hessian dimension is not unreasonably large.

```
EXIT -- 90 Input arguments out of range
```

INFO -- 91 invalid input argument

These conditions occur if some data associated with the problem is out of range.

For INFO 91, at least one input argument for the interface is invalid. The Print and Summary files provide more detail about which arguments must be modified.

5.5. Solution output

At the end of a run, the final solution is output to the Print file in accordance with the Solution keyword. Some header information appears first to identify the problem and the final state of the optimization procedure. A ROWS section and a COLUMNS section then follow, giving one line of information for each row and column. The format used is similar to certain commercial systems, though there is no industry standard.

An example of the printed solution is given in Section 5. In general, numerical values are output with format f16.5. The maximum record length is 111 characters, including the first (carriage-control) character.

To reduce clutter, a dot "." is printed for any numerical value that is exactly zero. The values ± 1 are also printed specially as 1.0 and -1.0. Infinite bounds ($\pm 10^{20}$ or larger) are printed as None.

Note: If two problems are the same except that one minimizes an objective $f_0(x)$ and the other maximizes $-f_0(x)$, their solutions will be the same but the signs of the dual variables π_i and the reduced gradients d_j will be reversed.

The ROWS section

General linear constraints take the form $l \leq Ax \leq u$. The *i*th constraint is therefore of the form

$$\alpha \leq a^T x \leq \beta$$
,

and the value of a^Tx is called the *row activity*. Internally, the linear constraints take the form Ax - s = 0, where the slack variables s should satisfy the bounds $l \le s \le u$. For the ith "row", it is the slack variable s_i that is directly available, and it is sometimes convenient to refer to its state. Slacks may be basic or nonbasic (but not superbasic).

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

Label Description

Number The value n+i. This is the internal number used to refer to the *i*th slack in the iteration log.

Row The name of the ith row.

State The state of the *i*th row relative to the bounds α and β . The various states possible are as follows.

LL The row is at its lower limit, α .

UL The row is at its upper limit, β .

EQ The limits are the same $(\alpha = \beta)$.

BS The constraint is not binding. s_i is basic.

A key is sometimes printed before the **State** to give some additional information about the state of the slack variable.

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

Note: If Scale option > 0, the tests for assigning A, D, I, N are made on the scaled problem because the keys are then more likely to be meaningful.

Activity The row value a^Tx (or $f_i(x) + a^Tx$ for nonlinear rows).

Slack activity The amount by which the row differs from its nearest bound. (For free rows, it is taken to be minus the Activity.)

Lower limit α , the lower bound on the row.

Upper limit β , the upper bound on the row.

Dual activity The value of the dual variable π_i , often called the shadow price (or simplex multiplier) for the *i*th constraint. The full vector π always satisfies $B^T\pi = g_B$, where B is the current basis matrix and g_B contains the associated gradients for the current objective function.

I The constraint number, i.

The COLUMNS section

Here we talk about the "column variables" x_j , j = 1: n. We assume that a typical variable has bounds $\alpha \leq x_j \leq \beta$.

Label Description

Number The column number, j. This is the internal number used to refer to x_j in the iteration log.

Column The name of x_i .

State The state of x_j relative to the bounds α and β . The various states possible are as follows.

LL x_i is nonbasic at its lower limit, α .

UL x_i is nonbasic at its upper limit, β .

EQ x_j is nonbasic and fixed at the value $\alpha = \beta$.

FR x_j is nonbasic at some value strictly between its bounds: $\alpha < x_j < \beta$.

BS x_j is basic. Usually $\alpha < x_j < \beta$.

SBS x_j is superbasic. Usually $\alpha < x_j < \beta$.

A key is sometimes printed before the State to give some additional information about the state of x_j .

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

Note: If Scale option > 0, the tests for assigning A, D, I, N are made on the scaled problem because the keys are then more likely to be meaningful.

Activity The value of the variable x_i .

Obj Gradient g_j , the jth component of the gradient of the (linear or nonlinear) objective function. (If any x_j is infeasible, g_j is the gradient of the sum of infeasibilities.)

Lower limit α , the lower bound on x_i .

Upper limit β , the upper bound on x_i .

Reduced gradnt The reduced gradient $d_j = g_j - \pi^T a_j$, where a_j is the *j*th column of the constraint matrix (or the *j*th column of the Jacobian at the start of the final major iteration).

M+J The value m+j.

Note: If two problems are the same except that one minimizes $f_0(x)$ and the other maximizes $-f_0(x)$, their solutions will be the same but the signs of the dual variables π_i and the reduced gradients d_i will be reversed.

5.6. The SOLUTION file

The information in a printed solution (Section 5.5) may be output as a Solution file, according to the Solution file option (which may refer to the Print file if so desired). Infinite bounds appear as $\pm 10^{20}$ rather than None. Other numerical values are output with format 1p, e16.6.

A Solution file is intended to be read from disk by a self-contained program that extracts and saves certain values as required for possible further computation. Typically the first 14 records would be ignored. Each subsequent record may be read using

```
format(i8, 2x, 2a4, 1x, a1, 1x, a3, 5e16.6, i7)
```

adapted to suit the occasion. The end of the ROWS section is marked by a record that starts with a 1 and is otherwise blank. If this and the next 4 records are skipped, the COLUMNS section can then be read under the same format. (There should be no need for backspace statements.)

5.7. The SUMMARY file

If Summary file > 0, the following information is output to the Summary file. (It is a brief form of the Print file.) All output lines are less than 72 characters.

- The Begin line from the Specs file, if any.
- The basis file loaded, if any.
- A brief Major iteration log.
- A brief Minor iteration log.
- The EXIT condition and a summary of the final solution.

The following Summary file is from the example of Section 3.2, using Major print level 1 and Minor print level 0.

```
N P S O L 2.0-1.0 (Sep 2013)
```

```
Begin Options for dnopt 1.00-2 sample problem.
DNSPEC
        EXIT 100 -- finished successfully
DNSPEC
        INFO 101 -- SPECS file read
Starting dntoy
The user has defined
                          3 out of
                                          4 constraint gradients.
==> Some constraint derivatives are missing, assumed constant.
                                           3 objective gradients.
The user has defined
                          3 out of
                       nCon Feasible Optimal MeritFunction
Major minors
                Step
                                                               nZ Penalty
                          1 4.0E+00 6.3E-01 0.0000000E+00
                                                               1
              3.3E-01
                          2 1.3E+00 2.6E-01 3.1576447E+01
   1
          1
                                                                1 4.0E+00
                                                                            rl
   2
              4.3E-01
                          3 5.0E-01 5.4E-01 2.9821036E+01
                                                                1 4.0E+00 s 1
          1
   3
          2
              1.0E+00
                          5 3.4E-02 1.3E+00 2.7256147E+01
                                                                2 4.0E+00 m
                          7 9.7E-02 1.5E+00 2.0513592E+01
   4
          2
              1.0E+00
                                                                1 4.0E+00 m
              4.9E-01
                         11 3.7E-01 1.7E+00 1.5092938E+01
                                                                1 4.0E+00 m
          1
             1.0E+00
                         12 1.8E-01 1.6E+00 3.0765667E+00
                                                                1 4.0E+00
   6
          1
   7
          1
              1.0E+00
                         14 1.7E-02 9.1E-01 3.6637505E+00
                                                                  3.2E+01
   8
          0
              1.0E+00
                         15 2.2E-02 3.4E-01 2.1167709E+00
                                                                  6.1E+00
             1.0E+00
                         16 4.5E-03 5.6E-02 1.9112081E+00
                                                                1 6.1E+00
   9
          1
Major minors
                       nCon Feasible Optimal MeritFunction
                                                               nZ Penalty
                Step
                         17 1.8E-04 6.3E-04 1.9001428E+00
  10
          1
              1.0E+00
                                                                1 6.1E+00
                         18 (7.2E-08) 1.1E-04 1.9001250E+00
  11
          1
              1.0E+00
                                                                1 6.1E+00
                         19 (1.6E-10) 5.8E-05 1.9001250E+00
              1.0E+00
                                                                1 6.1E+00
  12
          1
  13
             1.0E+00
                         20 (2.0E-10)(1.8E-09) 1.9001250E+00
                                                                1 6.1E+00
        EXIT 0 -- finished successfully INFO 1 -- optimality conditions satisfied
DNOPT
DNOPT
Problem name
No. of iterations
                                  16
                                       Objective value
                                                           1.9001249926E+00
No. of major iterations
                                  13
                                       Linear objective
                                                           9.9624996883E-02
                                      Nonlinear objective 1.8004999958E+00
                           6.080E+00
Penalty parameter
No. of calls to funobj
                                  21
                                       No. of calls to funcon
                                                                         21
Degrees of freedom
No. of degenerate steps
                                   0
                                      Percentage
                                                                       0.00
```

Finishing dntoy

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