NLPQLP: A New Fortran Implementation of a Sequential Quadratic Programming Algorithm for Parallel Computing

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Abstract

The Fortran subroutine NLPQLP solves smooth nonlinear programming problems and is an extension of the code NLPQL. The new version is specifically tuned to run under distributed systems. A new input parameter l is introduced for the number of parallel machines, that is the number of function calls to be executed simultaneously. In case of $l = 1$, NLPQLP is identical to NLPQL. Otherwise the line search is modified to allow parallel function calls either for the line search or for approximating gradients by difference formulae. The mathematical background is outlined, in particular the modification of line search algorithms to retain convergence under parallel systems. Numerical results show the sensitivity of the new version with respect to the number of parallel machines, and the influence of different gradient approximations under uncertainty. The performance evaluation is obtained by more than 300 standard test problems.

1 Introduction

We consider the general optimization problem, to minimize an objective function f under nonlinear equality and inequality constraints, i.e.

$$x \in I\!R^n : \begin{array}{ll} \min f(x) & \\ g_j(x) = 0 \,, & j = 1, \ldots, m_e \\ g_j(x) \geq 0 \,, & j = m_e + 1, \ldots, m \\ x_l \leq x \leq x_u & \end{array} \tag{1}$$

where x is an n-dimensional parameter vector. To facilitate the subsequent notation, we assume that upper and lower bounds x_u and x_l are not handled separately, i.e. that they are considered as general inequality constraints. Then we get the nonlinear programming problem

$$x \in I\!R^n : \begin{array}{ll} \min f(x) & \\ g_j(x) = 0 \,, & j = 1, \ldots, m_e \\ g_j(x) \geq 0 \,, & j = m_e + 1, \ldots, m \end{array} \tag{2}$$

called now NLP in abbreviated form. It is assumed that all problem functions $f(x)$ and $g_j(x)$, $j = 1, \ldots, m$, are continuously differentiable on the whole $I\!R^n$. But besides of this we do not suppose any further structure in the model functions.

Sequential quadratic programming methods are the standard general purpose algorithms for solving smooth nonlinear optimization problems, at least under the following assumptions:

- The problem is not too big.
- The functions and gradients can be evaluated with sufficiently high precision.
- The problem is smooth and well-scaled.

The code NLPQL of Schittkowski [28] is a Fortran implementation of a sequential quadratic programming (SQP) algorithm. The design of the numerical algorithm is founded on extensive comparative numerical tests of Schittkowski [21, 25, 23], Schittkowski et al. [34], Hock and Schittkowski [13], and on further theoretical investigations published in [22, 24, 26, 27]. The algorithm is extended to solve also nonlinear least squares problems efficiently, see [31], and to handle problems with very many constraints, cf. [32]. To conduct the numerical tests, a random test problem generator is developed for a major comparative study, see [21]. Two collections with more than 300 academic and real-life test problems are published in Hock and Schittkowski [13] and in Schittkowski [29]. These test examples are now part of the Cute test problem collection of Bongartz et al. [4]. More than 100 test problems based on a finite element formulation are collected for the comparative evaluation in Schittkowski et al. [34].

Moreover there exist hundreds of commercial and academic applications of NLPQL, for example

1. Mechanical structural optimization, see Schittkowski et al. [34] and Kneppe et al. [15],

2. Data fitting and optimal control of transdermal pharmaceutical systems, see Boderke et al. [1] or Blatt and Schittkowski [3],

3. Computation of optimal feed rates for tubular reactors, see Birk et al. [2],

4. Food drying in a convection oven, see Frias et al. [11],

5. Optimal design of horn radiators for satellite communication, see Hartwanger, Schittkowski, Wolf [10],

6. Receptor-ligand binding studies, see Schittkowski [33].

The very first version of NLQPL developed in 1981, is still included in the IMSL Library [30], but meanwhile outdated because of numerous improvements and corrections made since then. Actual versions of NLPQL are part of commercial redistributed optimization systems like

- ANSYS/POPT (CAD-FEM, Grafing) for structural optimization,
- STRUREL (RCP, Munich) for reliability analysis,
- TEMPO (OECD Reactor Project, Halden) for control of power plants,
- Microwave Office Suit (Applied Wave Research, El Segundo) for electronic design,
- MOOROPT (Marintec, Trondheim) for the design of mooring systems,
- iSIGHT (Enginious Software, Cary, North Carolina) for multi-disciplinary CAE,
- POINTER (Synaps, Atlanta) for design automation.

Customers include Axiva, BASF, Bayer, Bell Labs, Chevron Research, DLR, Dornier Systems, Dow Chemical, EADS, ENSIGC, EPCOS, ESOC, Eurocopter, Fantoft Prosess, General Electric, GLM Lasertechnik, Hoechst, IABG, IBM, INRIA, INRS-Telecommunications, Mecalog, MTU, NASA, Nevesbu, NLR, Norsk Hydro Research, Numerola, Peaktime, Philips, Rolls-Royce, SAQ Kontroll, SDRC, Siemens, TNO, Transpower, US Air Force, and in addition dozens of academic research institutions all over the world.

The general availability of parallel computers and in particular of distributed computing through networks motivates a careful redesign of NLPQL, to allow simultaneous function calls with predetermined arguments. The resulting code is called NLPQLP and its mathematical background and usage is documented in this paper.

The iterative process of an SQP algorithm is highly sequential. Proceeding from a given initial design, new iterates are computed based only on the information available from the previous iterate. Each step requires the evaluation of all model functions $f(x_k)$ and $g_j(x_k)$, $j = 1, \ldots, m$, and of gradients $\nabla f(x_k)$ and $\nabla g_j(x_k)$,

$j \in J_k$. x_k is the current iterate and $J_k \subset \{1, \ldots, m\}$ a suitable active set determined by the algorithm.

The most effective possibility to exploit a parallel system architecture occurs, when gradients cannot be calculated analytically, but have to be approximated numerically, for example by forward differences, two-sided differences, or even higher order methods. Then we need at least n additional function calls, where n is the number of optimization variables, or a suitable multiple of n. Assuming now that a parallel computing environment is available with l processors, we need only one simultaneous function evaluation in each iteration for getting the gradients, if $l \geq n$. In the most simple case, we have to execute the given simulation program to get $f(x_k + h_{ik}e_i)$ and $g_j(x_k + h_{ik}e_i)$, $j = 1, \ldots, m$, for all $i = 1, \ldots, n$, on n different processors, where h_{ik} is a small perturbation of the i-th unit vector scaled by the actual value of the i-th coefficient of x_k. Subsequently the partial derivatives are approximated by forward differences

$$\frac{1}{h_{ik}}(f(x_k + h_{ik}e_i) - f(x_k)) \quad , \qquad \frac{1}{h_{ik}}(g_j(x_k + h_{ik}e_i) - g_j(x_k))$$

for $j \in J_k$. Two-sided differences can be used, if $2n \leq l$, fourth-order differences in case of $4n \leq l$, etc.

Another reason for an SQP code to require function evaluations, is the line search. Based on the gradient information at an actual iterate $x_k \in I\!R^n$, a quadratic programming (QP) problem is formulated and solved to get a search direction $d_k \in I\!R^n$. It must be ensured that the solution of the QP is a descent direction subject to a certain merit function. Then a sequential line search along $x_k + \alpha d_k$ is performed by combining quadratic interpolation and a steplength reduction. The iteration is stopped as soon as a sufficient descent property is satisfied, leading to a steplength α_k and a new iterate $x_{k+1} = x_k + \alpha_k d_k$. We know that the line search can be restricted to the interval $0 < \alpha \leq 1$, since $\alpha_k = 1$ is expected close to a solution, see e.g. Spellucci [35], because of the local superlinear convergence of an SQP algorithm. Thus, the line search is always started at $\alpha = 1$.

To outline the new approach, let us assume that functions can be computed simultaneously on l different machines. Then l test values $\alpha^i = \beta^{i-1}$ with $\beta = \epsilon^{1/(l-1)}$ are selected, $i = 1, \ldots, l$, where ϵ is a guess for the machine precision. Next we require l parallel function calls to get the corresponding model function values. The first α^i satisfying a sufficient descent property, is accepted as the new steplength for getting the subsequent iterate. One has to be sure, that existing convergence results of the SQP algorithm are not violated. For an alternative approach based on pattern search, see Hough, Kolda, and Torczon [14].

The parallel model of parallelism is SPMD, i.e., Single Program Multiple Data. In a typical situation we suppose that there is a complex application code providing simulation data, for example by an expensive finite element calculation. It is supposed that various instances of the simulation code providing function values, are executable on a series of different machines, so-called slaves, controlled by a

master program that executes NLPQLP. By a message passing system, for example PVM, see Geist et al. [6], only very few data need to be transferred from the master to the slaves. Typically only a set of design parameters of length n must to be passed. On return, the master accepts new model responses for objective function and constraints, at most $m + 1$ double precision numbers. All massive numerical calculations and model data, for example all FE data, remain on the slave processors of the distributed system.

The investigations of this paper do not require a special parallel system architecture. We present only a variant of an existing SQP code for nonlinear programming, that can be embedded into an arbitrary distributed environment. A realistic implementation depends highly on available hardware, operating system, or virtual machine, and particularly on the underlying simulation package by which function values are to be computed.

In Section 2 we outline the general mathematical structure of an SQP algorithm, and consider some details of quasi-Newton updates and merit functions in Section 3. Sequential and parallel line search algorithms are described in Section 4. It is shown how the traditional approach is replaced by a more restrictive one with predetermined simultaneous function calls, nevertheless guaranteeing convergence. Numerical results are summarized in Section 5. First it is shown, how the parallel execution of the merit function depends on the number of available machines. Also we compare the results with those obtained by full sequential line search. Since parallel function evaluations are highly valuable in case of numerical gradient computations, we compare also the effect of several difference formulae. Model functions are often disturbed in practical environments, for example in case of iterative algorithms required for internal auxiliary computations. Thus, we add random errors to simulate uncertainties in function evaluations, and compare the overall efficiency of an SQP algorithm. The usage of the Fortran subroutine is documented in Section 6 together with an illustrative example.

2 Sequential Quadratic Programming Methods

Sequential quadratic programming or SQP methods belong to the most powerful nonlinear programming algorithms we know today for solving differentiable nonlinear programming problems of the form (1) or (2), respectively. The theoretical background is described e.g. in Stoer [36] in form of a review, or in Spellucci [35] in form of an extensive text book. From the more practical point of view SQP methods are also introduced briefly in the books of Papalambros, Wilde [17] and Edgar, Himmelblau [5]. Their excellent numerical performance was tested and compared with other methods in Schittkowski [21], and since many years they belong to the most frequently used algorithms to solve practical optimization problems.

The basic idea is to formulate and solve a quadratic programming subproblem in each iteration which is obtained by linearizing the constraints and approximating

the Lagrangian function

$$L(x,u) := f(x) - \sum_{j=1}^{m} u_j g_j(x) \tag{3}$$

quadratically, where $x \in I\!R^n$, and where $u = (u_1, \ldots, u_m)^T \in I\!R^m$ is the multiplier vector.

To formulate the quadratic programming subproblem, we proceed from given iterates $x_k \in I\!R^n$, an approximation of the solution, $v_k \in I\!R^m$ an approximation of the multipliers, and $B_k \in I\!R^{n\times n}$, an approximation of the Hessian of the Lagrangian function. Then one has to solve the following quadratic programming problem:

$$\begin{aligned} & \min \tfrac{1}{2} d^T B_k d + \nabla f(x_k)^T d \\ d \in I\!R^n: \quad & \nabla g_j(x_k)^T d + g_j(x_k) = 0\ , \quad j = 1, \ldots, m_e\ , \\ & \nabla g_j(x_k)^T d + g_j(x_k) \geq 0\ , \quad j = m_e+1, \ldots, m\ . \end{aligned} \tag{4}$$

It is supposed that bounds are not available or included as general inequality constraints to simplify the notation. Otherwise we proceed from (2) and pass the bounds to the quadratic program directly. Let d_k be the optimal solution and u_k the corresponding multiplier. A new iterate is obtained by

$$\begin{pmatrix} x_{k+1} \\ v_{k+1} \end{pmatrix} := \begin{pmatrix} x_k \\ v_k \end{pmatrix} + \alpha_k \begin{pmatrix} d_k \\ u_k - v_k \end{pmatrix}\ , \tag{5}$$

where $\alpha_k \in (0,1]$ is a suitable steplength parameter.

The motivation for the success of SQP methods is found in the following observation: An SQP method is identical to Newton's method to solve the necessary optimality conditions, if B_k is the Hessian of the Lagrangian function and if we start sufficiently close to a solution. The statement is easily derived in case of equality constraints only, that is $m_e = m$, but holds also for inequality restrictions. A straightforward analysis shows that if $d_k = 0$ is an optimal solution of (4) and u_k the corresponding multiplier vector, then x_k and u_k satisfy the necessary optimality conditions of (2).

Although we are able to guarantee that the matrix B_k is positive definite, it is possible that (4) is not solvable due to inconsistent constraints. One possible remedy is to introduce an additional variable $\delta \in I\!R$, leading to the modified problem

$$\begin{aligned} & \min \tfrac{1}{2} d^T B_k d + \nabla f(x_k)^T d + \sigma_k \delta^2 \\ d \in I\!R^n, \quad & \nabla g_j(x_k)^T d + (1-\delta) g_j(x_k) \left\{ \begin{matrix} = \\ \geq \end{matrix} \right\} 0, \quad j \in J_k\ , \\ \delta \in I\!R: \quad & \nabla g_j(x_{k(j)})^T d + g_j(x_k) \geq 0, \qquad\qquad j \in K_k \\ & 0 \leq \delta \leq 1\ . \end{aligned} \tag{6}$$

σ_k is a suitable penalty parameter to force that the influence of the additionally introduced variable δ is as small as possible, cf. Schittkowski [26] for details. The

active set J_k is given by

$$J_k := \{1, \ldots, m_e\} \cup \{j : m_e < j \leq m,\ g_j(x_k) < \epsilon \quad \text{or} \quad u_j^k > 0\} \tag{7}$$

and K_k is the complement, i.e. $K_k := \{1, \ldots, m\} \backslash J_k$.

In (7), ϵ is any small tolerance to define the active constraints, and u_j^k denotes the j-th coefficient of u_k. Obviously, the point $d_0 = 0$, $\delta_0 = 1$ satisfies the linear constraints of (6) which is then always solvable. Moreover it is possible to avoid unnecessary gradient evaluations by recalculating only those gradients of restriction functions, that belong to the active set, as indicated by the index '$k(j)$'.

3 Merit Functions and Quasi-Newton Updates

The steplength parameter α_k is required in (5) to enforce global convergence of the SQP method, i.e. the approximation of a point satisfying the necessary Karush-Kuhn-Tucker optimality conditions when starting from arbitrary initial values, e.g. a user-provided $x_0 \in I\!R^n$ and $v_0 = 0$, $B_0 = I$. α_k should satisfy at least a sufficient decrease of a merit function $\phi_r(\alpha)$ given by

$$\phi_r(\alpha) := \psi_r \left(\begin{pmatrix} x \\ v \end{pmatrix} + \alpha \begin{pmatrix} d \\ u - v \end{pmatrix} \right) \tag{8}$$

with a suitable penalty function $\psi_r(x, v)$. Possible choices of ψ_r are the L_1-penalty function

$$\psi_r(x, v) := f(x) + \sum_{j=1}^{m_e} r_j |g_j(x)| + \sum_{j=m_e+1}^{m} r_j |\min(0, g_j(x))| \ , \tag{9}$$

cf. Han [9] and Powell [18], or the augmented Lagrangian function

$$\psi_r(x, v) := f(x) - \sum_{j \in J} (v_j g_j(x) - \frac{1}{2} r_j g_j(x)^2) - \frac{1}{2} \sum_{j \in K} v_j^2 / r_j \ , \tag{10}$$

with $J := \{1, \ldots, m_e\} \cup \{j : m_e < j \leq m, g_j(x) \leq v_j / r_j\}$ and $K := \{1, \ldots, m\} \setminus J$, cf. Schittkowski [26]. In both cases the objective function is *penalized* as soon as an iterate leaves the feasible domain.

The corresponding penalty parameters that control the degree of constraint violation, must be chosen in a suitable way to guarantee a descent direction of the merit function. Possible choices are

$$r_j^{(k)} := \max(|u_j^{(k)}| \ , \ \frac{1}{2}(r_j^{(k-1)} + |u_j^{(k)}|) \ ,$$

see Powell [18] for the L_1-merit function (9), or

$$r_j^{(k)} := \max \left(\frac{2m(u_j^{(k)} - v_j^{(k)^2}}{(1 - \delta_k) d_k^T B_k d_k} \ , r_j^{(k-1)} \right) \tag{11}$$

for the augmented Lagrangian function (10), see Schittkowski [26].

Here δ_k is the additionally introduced variable to avoid inconsistent quadratic programming problems, see (6). For both merit functions we get the following descent property that is essential to prove convergence:

$$\phi'_{r_k}(0) = \bigtriangledown \psi_{r_k}(x_k, v_k)^T \begin{pmatrix} d_k \\ u_k - v_k \end{pmatrix} < 0 \tag{12}$$

For the proof see Han [9] or Schittkowski [26].

Finally one has to approximate the Hessian matrix of the Lagrangian function in a suitable way. To avoid calculation of second derivatives and to obtain a final superlinear convergence rate, the standard approach is to update B_k by the BFGS quasi-Newton formula, cf. Powell [19] or Stoer [36]. The calculation of any new matrix B_{k+1} depends only on B_k and two vectors

$$\begin{array}{rcl} q_k & := & \nabla_x L(x_{k+1}, u_k) - \nabla_x L(x_k, u_k) \ , \\ w_k & := & x_{k+1} - x_k \ , \end{array} \tag{13}$$

i.e.

$$B_{k+1} := \Pi(B_k, q_k, w_k) \ , \tag{14}$$

where

$$\Pi(B, q, w) := B + \frac{qq^T}{q^T w} - \frac{Bww^T B}{w^T B w} \ . \tag{15}$$

The above formula yields a positive definite matrix B_{k+1} provided that B_k is positive definite and $q_k^T w_k > 0$. A simple modification of Powell [18] guarantees positive definite matrices even if the latter condition is violated.

There remains the question whether the convergence of an SQP method can be proved in a mathematically rigorous way. In fact there exist numerous theoretical convergence results in the literature, see e.g. Spellucci [35]. We want to give here only an impression about the type of these statements, and repeat two results that have been stated in the early days of the SQP methods.

In the first case we consider the global convergence behaviour, i.e. the question, whether the SQP methods converges when starting from an arbitrary initial point. Suppose that the augmented Lagrangian merit function (8) is implemented and that the primal and dual variables are updated in the form (10).

Theorem 3.1 *Let $\{(x_k, v_k)\}$ be a bounded iteration sequence of the SQP algorithm with a bounded sequence of quasi-Newton matrices $\{B_k\}$ and assume that there are positive constants γ and $\overline{\delta}$ with*

(i) $d_k^T B_k d_k \geq \gamma d_k^T d_k$ *for all* k *and a* $\gamma > 0$,

(ii) $\delta_k \leq \overline{\delta}$ *for all* k,

(iii) $\sigma_k \geq \|A(x_k)v_k\|^2 / \gamma(1 - \overline{\delta})^2$ *for all* k,

Then there exists an accumulation point of $\{(x_k, v_k)\}$ *satisfying the Karush-Kuhn-Tucker conditions for (2).*

Assumption (i) is very well known from unconstrained optimization. It says that the angles between the steepest descent directions and the search directions obtained from the quadratic programming subproblems, must be bounded away from $\pi/2$. Assumptions (ii) and (iii) are a bit more technical and serve to control the additionally introduced variable δ for preventing inconsistency.

The proof of the theorem is found in Schittkowski [26]. The statement is quite weak, but without any further information about second derivatives, we cannot guarantee that the approximated point is indeed a local minimizer.

To investigate now the local convergence speed, we assume that we start from an initial point x_0 sufficiently close to an optimal solution. General assumptions for local convergence analysis are:

a) $z^\star = (x^\star, u^\star)$ is a strong local minimizer of (2).

b) $m_e = m$, i.e. we know all active constraints.

c) f, g_1, ..., g_m are twice continuously differentiable.

d) For $z_k := (x_k, v_k)$ we have $\lim_{k\to\infty} z_k = z^\star$.

e) The gradients $\bigtriangledown g_1(x^\star)$, ..., $\bigtriangledown g_m(x^\star)$ are linearly independent, i.e. the constraint qualification is satisfied.

f) $d^T B_k d \geq \gamma d^T d$ for all $d \in R^n$ with $A(x_k)^T d = 0$, i.e. some kind of second order condition for the Hessian approximation.

Powell [19] proved the following theorem for the BFGS update formula:

Theorem 3.2 *Assume that*

(i) $\bigtriangledown_x^2 L(x^\star, u^\star)$ *is positive definite,*

(ii) $\alpha_k = 1$ *for all* k,

then the sequence $\{x_k\}$ *converges R-superlinearly, i.e.*

$$\lim_{k\to\infty} \|x_{k+1} - x^\star\|^{1/k} = 0 \quad .$$

The R-superlinear convergence speed is somewhat weaker than the Q-superlinear convergence rate defined below. It was Han [8] who proved the statement

$$\lim_{k\to\infty} \frac{\|z_{k+1} - z^\star\|}{\|z_k - z^\star\|} = 0 \quad .$$

for the so-called DFP update formula, i.e. a slightly different quasi-Newton method. In this case, we get a sequence β_k tending to zero with

$$\|z_{k+1} - z^\star\| \leq \beta_k \|z_k - z^\star\|$$

4 Steplength Calculation

Let us consider in more detail, how a steplength α_k is actually calculated. First we select a suitable merit function, in our case the augmented Lagrangian (10), that defines a scalar function $\phi_r(\alpha)$. For obvious reasons, a full minimization along α is not possible. The idea is to get a sufficient decrease for example measured by the so-called Goldstein condition

$$\phi_r(0) + \alpha\mu_2\phi_r'(0) \leq \phi_r(\alpha) \leq \phi_r(0) + \alpha\mu_1\phi_r'(0) \tag{16}$$

or the Armijo condition

$$\phi_r(\sigma\beta^i) \leq \phi_r(0) + \sigma\beta^i\mu\phi_r'(0) \quad , \tag{17}$$

see for example Ortega and Rheinboldt [16]. The constants are from the ranges $0 < \mu_1 \leq 0.5 < \mu_2 < 1$, $0 < \mu < 0.5$, $0 < \beta < 1$, and $0 < \sigma \leq 1$. In the first case, we accept any α in the range given by (16), whereas the second condition is constructive. We start with $i = 0$ and increase i, until (17) is satisfied for the first time, say at i_k. Then the desired steplength is $\alpha_k = \sigma\beta^{i_k}$. Both approaches are feasible because of the descent property $\phi_r'(0) < 0$, see (12).

All line search algorithms have to satisfy two requirements, which are somewhat contradicting:

1. The decrease of the merit function must be sufficiently large, to accelerate convergence.

2. The steplength must not become too small to avoid convergence against a non-stationary point.

The implementation of a line search algorithm is a critical issue when implementing a nonlinear programming algorithm, and has significant effect on the overall efficiency of the resulting code. On the one hand we need a line search to stabilize the algorithm, on the other hand it is not advisable to waste too many function calls. Moreover the behaviour of the merit function becomes irregular in case on constrained optimization, because of very steep slopes at the border caused by the penalty terms. Even the implementation is more complex than shown above, if linear constraints and bounds of the variables are to be satisfied during the line search.

Fortunately SQP methods are quite robust and accept the steplength one in the neighborhood of a solution. Typically the test parameter μ for the Armijo-type sufficient descent property (17) is very small, for example $\mu = 0.0001$ in the present implementation of NLPQL. Nevertheless the choice of the reduction parameter β must be adopted to the actual slope of the merit function. If β is too small, the line search terminates very fast, but on the other hand the resulting stepsizes are usually too small leading to a higher number of outer iterations. On the other hand, a larger

value close to one requires too many function calls during the line search. Thus, we need some kind of compromise, which is obtained by applying first a polynomial interpolation, typically a quadratic one, and use (16) or (17) only as a stopping criterion. Since $\phi_r(0)$, $\phi_r'(0)$, and $\phi_r(\alpha_i)$ are given, α_i the actual iterate of the line search procedure, we get easily the minimizer of the quadratic interpolation. We accept then the maximum of this value or the Armijo parameter as a new iterate, as shown by the subsequent code fragment implemented in NLPQL:

Algorithm 4.1:

Let β, μ with $0 < \beta < 1$, $0 < \mu < 0.5$ be given.

Start: $\alpha_0 := 1$

For $i = 0, 1, 2, \ldots$ do

1) If $\phi_r(\alpha_i) < \phi_r(0) + \mu\alpha_i\phi_r'(0)$, then stop.

2) Compute $\bar{\alpha}_i := 0.5\alpha_i^2\phi_r'(0)/(\alpha_i\phi_r'(0) - \phi_r(\alpha_i) + \phi_r(0))$.

3) Let $\alpha_{i+1} := \max(\beta\alpha_i, \bar{\alpha}_i)$.

Corresponding convergence results are found in Schittkowski [26]. $\bar{\alpha}_i$ is the minimizer of the quadratic interpolation, and we use the Armijo descent property for termination. Step 3) is required to avoid irregular values, since the minimizer of the quadratic interpolation may reside outside of the feasible domain $(0, 1]$. The search algorithm is implemented in NLPQL together with additional safeguards, for example to prevent violation of bounds. Algorithm 4.1 assumes that $\phi_r(1)$ is known before calling the procedure, i.e., the corresponding function call is made in the calling program. We have to stop the algorithm, if sufficient descent is not observed after a certain number of iterations, say 10. If the tested stepsizes fall below machine precision or the accuracy by which model function values are computed, the merit function cannot decrease further.

Now we come back to the question, how the sequential line search algorithm can be modified to work under a parallel computing environment. Proceeding from an existing implementation as outlined above, the answer is quite simple. To outline the new approach, let us assume that functions can be computed simultaneously on l different machines. Then l test values $\alpha_i = \beta^i$ with $\beta = \epsilon^{1/(l-1)}$ are selected, $i = 0$, ..., $l - 1$, where ϵ is a guess for the machine precision. Next we order l parallel function calls to get $f(x_k + \alpha^i d_k)$ and $g_j(x_k + \alpha^i d_k)$, $j = 1$, ..., m, for $i = 0$, ..., $l - 1$. The first α^i satisfying the sufficient descent property (17), is accepted as the steplength for getting the subsequent iterate x_{k+1}.

The proposed parallel line search will work efficiently, if the number of parallel machines l is sufficiently large, and is summarized as follows:

Algorithm 4.2:

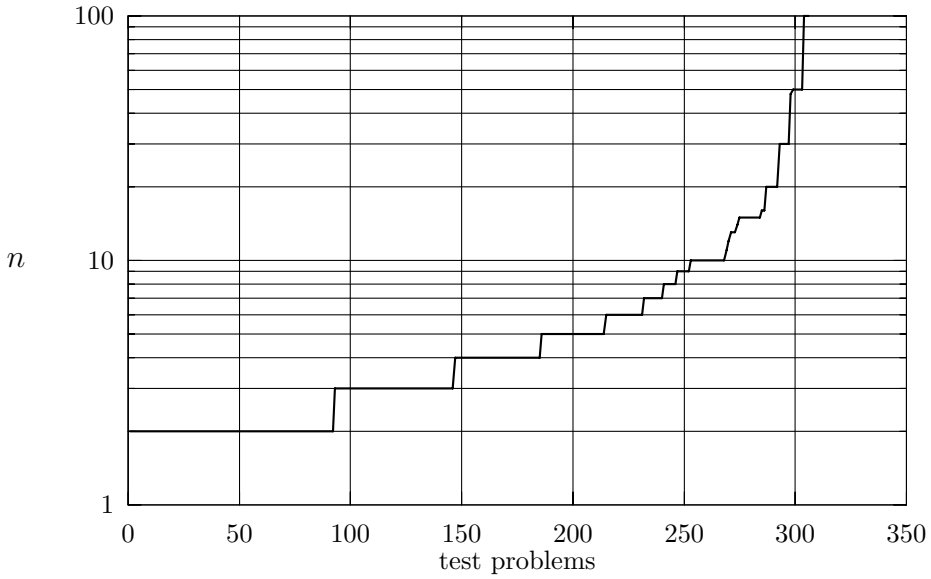

Figure 1: Number of Variables

Let β, μ with $0 < \beta < 1$, $0 < \mu < 0.5$ be given.

Start: For $\alpha_i = \beta^i$ compute $\phi_r(\alpha_i)$ for $i = 0, \ldots, l-1$.

For $i = 0, 1, 2, \ldots$ do

1) If $\phi_r(\alpha_i) < \phi_r(0) + \mu\alpha_i\phi_r'(0)$, then stop.

2) Let $\alpha_{i+1} := \beta\alpha_i$.

5 Numerical Results

Our numerical tests use all 306 academic and real-life test problems published in Hock and Schittkowski [13] and in Schittkowski [29]. The distribution of the dimension parameter n, the number of variables, is shown in Figure 1. We see, for example, that about 270 of 306 test problems have not more than 10 variables. In a similar way, the distribution of the number of constraints is shown in Figure 2.

Since analytical derivatives are not available for all problems, we approximate them numerically. The test examples are provided with exact solutions, either known from analytical solutions or from the best numerical data found so far. The Fortran code is compiled by the Compaq Visual Fortran Optimizing Compiler, Version 6.5, under Windows 2000, and executed on a Pentium III processor with 750 MHz. Since the calculation times are very short, about 15 sec for solving all 306 test problems, we count only function and gradient evaluations. This is a realistic assumption, since for the practical applications in mind calculation times for evaluating model functions, dominate and the numerical efforts within NLPQLP are negligible.

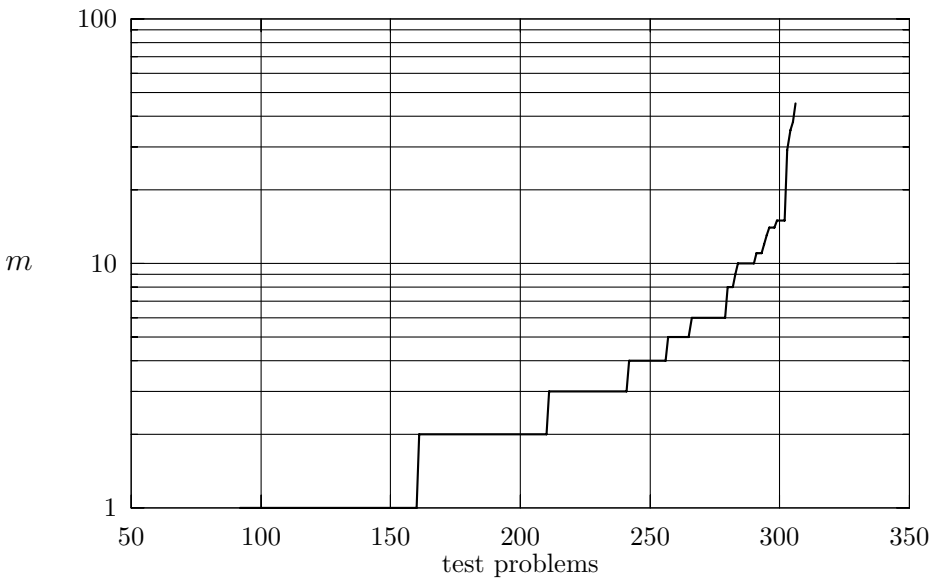

Figure 2: Number of Constraints

First we need a criterion to decide, whether the result of a test run is considered as a successful return or not. Let $\epsilon > 0$ be a tolerance for defining the relative termination accuracy, x_k the final iterate of a test run, and $x^\star$ the supposed exact solution as reported by the two test problem collections. Then we call the output of an execution of NLPQLP a successful return, if the relative error in objective function is less than ϵ and if the sum of all constraint violations less than ϵ^2, i.e., if

$$f(x_k) - f(x^\star) < \epsilon |f(x^\star)| \ , \ \text{if } f(x^\star) <> 0 \ \ ,$$

or

$$f(x_k) < \epsilon \ , \ \text{if } f(x^\star) = 0 \ \ ,$$

and

$$r(x_k) := \sum_{j=1}^{m_e} |g_j(x_k)| + \sum_{j=m_e+1}^{m} |\min(0, g_j(x_k))| < \epsilon^2 \ \ .$$

We take into account that NLPQLP returns a solution with a better function value than the known one, subject to the error tolerance of the allowed constraint violation. However there is still the possibility that NLPQLP terminates at a local solution different from the one known in advance. Thus, we call a test run a successful one, if NLPQLP terminates with error message *IFAIL=0*, and if

$$f(x_k) - f(x^\star) \geq \epsilon |f(x^\star)| \ , \ \text{if } f(x^\star) <> 0 \ \ ,$$

or

$$f(x_k) \geq \epsilon \ , \ \text{if } f(x^\star) = 0 \ \ ,$$

L	SUCC	NF	NIT
1	305	41	26
3	205	709	178
4	250	624	125
5	281	470	79
6	290	339	49
7	291	323	41
8	296	299	34
9	298	305	31
10	299	300	28
12	300	346	27
15	296	394	25
20	298	519	25
50	299	1,280	25

Table 1: Performance Results for Parallel Line Search

and

$$r(x_k) < \epsilon^2 \quad .$$

For our numerical tests, we use $\epsilon = 0.01$, i.e., we require a final accuracy of one per cent. NLPQLP is executed with termination accuracy ACC=10^{-8}, and *MAXIT=500*. Gradients are approximated by a fourth-order difference formula

$$\frac{\partial}{\partial x_i} f(x) \approx \frac{1}{4!\eta_i}\Big(2f(x-2\eta_i e_i) - 16f(x-\eta_i e_i) + 16f(x+\eta_i e_i) - 2f(x+2\eta_i e_i)\Big) \quad , \quad (18)$$

where $\eta_i = \eta \max(10^{-5}, |x_i|)$, $\eta = 10^{-7}$, e_i the i-th unit vector, and $i = 1, \ldots, n$. In a similar way, derivatives of the constraint functions are computed.

First we investigate the question, how the parallel line search influences the overall performance. Table 1 shows the number of successful test runs *SUCC*, the average number of function calls *NF*, and the average number of iterations *NIT*, for increasing number of simulated parallel calls of model functions denoted by L. To get *NF*, we count each single function call, also in the case $L > 1$. However, function evaluations needed for gradient approximations, are not counted. Their average number is *4*×*NIT*.

$L = 1$ corresponds to the sequential case, when Algorithm 4.1 is applied for the line search, consisting of a quadratic interpolation combined with an Armijo-type bisection strategy. Only one problem, TP108, could not be solved successfully, since a necessary regularity assumption called constraint qualification is violated at the optimal solution. Since we need at least one function evaluation for the subsequent iterate, we observe that the average number of additional function evaluations needed for the line search, is less than one.

In all other cases, $L > 1$ simultaneous function evaluations are made according to Algorithm 4.2. Thus, the total number of function calls NF is quite big in Table 1. If, however, the number of parallel machines L is sufficiently large in a practical situation, we need only one simultaneous function evaluation in each step of the SQP algorithm. To get a reliable and robust line search, we need at least 5 parallel processors. No significant improvements are observed, if we have more than 10 parallel function evaluations.

The most promising possibility to exploit a parallel system architecture occurs, when gradients cannot be calculated analytically, but have to be approximated numerically, for example by forward differences, two-sided differences, or even higher order methods. Then we need at least n additional function calls, where n is the number of optimization variables, or a suitable multiple of n.

For our numerical tests, we implement 6 different approximation routines for derivatives. The first three are standard difference formulae of increasing order, the final three linear and quadratic approximations to attempt to eliminate the influence of round-off errors:

1. Forward differences:

$$\frac{\partial}{\partial x_i} f(x) \approx \frac{1}{\eta_i}(f(x + \eta_i e_i) - f(x))$$

2. Two-sided differences:

$$\frac{\partial}{\partial x_i} f(x) \approx \frac{1}{2\eta_i}(f(x + \eta_i e_i) - f(x - \eta_i e_i)$$

3. Fourth-order formula:

$$\frac{\partial}{\partial x_i} f(x) \approx \frac{1}{4!\eta_i}(2f(x - 2\eta_i e_i) - 16f(x - \eta_i e_i) + 16f(x + \eta_i e_i) - 2f(x + 2\eta_i e_i))$$

4. Three-point linear approximation:

$$\min_{a,b \in I\!R} \sum_{r=-1}^{1} (a + b(x_i + r\eta_i) - f(x + r\eta_i e_i))^2 \ , \frac{\partial}{\partial x_i} f(x) \approx b$$

5. Five-point quadratic approximation:

$$\min_{a,b,c \in I\!R} \sum_{r=-2}^{2} (a + b(x_i + r\eta_i) + c(x_i + r\eta_i))^2 - f(x + r\eta_i e_i)^2 \ , \frac{\partial}{\partial x_i} f(x) \approx b + 2cx_i$$

6. Five-point linear approximation:

$$\min_{a,b \in I\!R} \sum_{r=-2}^{2} (a + b(x_i + r\eta_i) - f(x_i + r\eta_i e_i))^2 \ , \frac{\partial}{\partial x_i} f(x) \approx b$$

		ETA=1E-7		ETA=5E-4		ETA=1E-2	
GA	ERR	SUCC	NIT	SUCC	NIT	SUCC	NIT
1	0.0	**294**	29	268	25	205	22
2	0.0	**300**	29	291	25	277	22
3	0.0	**299**	29	290	24	277	22
4	0.0	89	33	283	23	275	22
5	0.0	118	30	247	32	272	22
6	0.0	127	28	278	22	273	22
1	10^{-10}	203	32	263	24	195	25
2	10^{-10}	215	33	**289**	25	273	23
3	10^{-10}	220	34	**287**	25	278	23
4	10^{-10}	94	34	277	23	276	23
5	10^{-10}	121	33	254	29	275	23
6	10^{-10}	106	32	**284**	24	274	23
1	10^{-8}	121	35	250	26	194	25
2	10^{-8}	140	31	**270**	26	262	24
3	10^{-8}	125	35	260	28	**269**	24
4	10^{-8}	76	40	267	24	265	24
5	10^{-8}	124	33	244	33	260	24
6	10^{-8}	119	33	**273**	26	268	24
1	10^{-6}	11	115	208	28	172	27
2	10^{-6}	12	109	202	28	236	25
3	10^{-6}	17	74	217	26	**237**	26
4	10^{-6}	19	73	209	28	235	25
5	10^{-6}	38	47	220	33	**237**	25
6	10^{-6}	27	56	225	29	**242**	24

Table 2: Performance Results for Different Gradient Approximations

In the above formulae, $i = 1, \ldots, n$ is the index of the variables for which a partial derivative is to be computed, $x = (x_1, \ldots, x_n)^T$ the argument, e_i the i-the unit vector, and $\eta_i = \eta \max(10^{-5}, |x_i|)$ the relative perturbation. In the same way, derivatives for constraints are approximated.

Table 2 shows the corresponding results for the six different procedures under consideration (GA), and for increasing random perturbations (ERR). In particular we are interested in the number of successful runs for three different perturbations η (ETA). The termination tolerance of NLPQLP is set to ACC=*0.01* $\times$ ETA. Bold entries show the three best gradient approximations. The number of simulated parallel machines is set to 10.

6 Program Documentation

NLPQLP is implemented in form of a Fortran subroutine. The quadratic programming problem is solved by the code QL of the author, an implementation of the primal-dual method of Goldfarb and Idnani [7] going back to Powell [20]. Model functions and gradients are called by reverse communication.

Usage:

```
      CALL  NLPQLP(L,M,ME,MMAX,N,NMAX,MNN2,X,F,G,DF,DG,U,XL,XU,
     /      C,D,ACC,MAXFUN,MAXIT,IPRINT,MODE,IOUT,IFAIL,WA,LWA,
     /      KWA,LKWA,ACTIVE,LACTIV,QP)
```

Definition of the parameters:

L :	Number of parallel systems, i.e. function calls during line search at predetermined iterates.
M :	Total number of constraints.
ME :	Number of equality constraints.
MMAX :	Row dimension of array DG containing Jacobian of constraints. MMAX must be at least one and greater or equal to M.
N :	Number of optimization variables.
NMAX :	Row dimension of C. NMAX must be at least two and greater than N.
MNN2 :	Must be equal to M+N+N+2 when calling NLPQLP.
X(NMAX,L) :	Initially, the first column of X has to contain starting values for the optimal solution. On return, X is replaced by the current iterate. In the driving program the row dimension of X has to be equal to NMAX. X is used internally to store L different arguments for which function values should be computed simultaneously.
F(L) :	On return, F(1) contains the final objective function value. F is used also to store L different objective function values to be computed from L iterates stored in X.
G(MMAX,L) :	On return, the first column of G contains the constraint function values at the final iterate X. In the driving program the row dimension of G has to be equal to MMAX. G is used internally to store L different set of constraint function values to be computed from L iterates stored in X.

DF(NMAX) :	DF contains the current gradient of the objective function. In case of numerical differentiation and a distributed system (L>1), it is recommended to apply parallel evaluations of F to compute DF.
DG(MMAX,NMAX) :	DG contains the gradients of the active constraints (ACTIVE(J)=.true.) at a current iterate X. The remaining rows are filled with previously computed gradients. In the driving program the row dimension of DG has to be equal to MMAX.
U(MNN2) :	U contains the multipliers with respect to the actual iterate stored in the first column of X. The first M locations contain the multipliers of the M nonlinear constraints, the subsequent N locations the multipliers of the lower bounds, and the final N locations the multipliers of the upper bounds. At an optimal solution, all multipliers with respect to inequality constraints should be nonnegative.
XL(N),XU(N) :	On input, the one-dimensional arrays XL and XU must contain the upper and lower bounds of the variables.
C(NMAX,NMAX) :	On return, C contains the last computed approximation of the Hessian matrix of the Lagrangian function stored in form of an Cholesky decomposition. C contains the lower triangular factor of an LDL factorization of the final quasi-Newton matrix (without diagonal elements, which are always one). In the driving program, the row dimension of C has to be equal to NMAX.
D(NMAX) :	The elements of the diagonal matrix of the LDL decomposition of the quasi-Newton matrix are stored in the one-dimensional array D.
ACC :	The user has to specify the desired final accuracy (e.g. 1.0D-7). The termination accuracy should not be much smaller than the accuracy by which gradients are computed.
STPMIN :	Minimum steplength in case of L>1. Recommended is any value in the order of the accuracy by which functions are computed.
MAXFUN :	The integer variable defines an upper bound for the number of function calls during the line search (e.g. 20). MAXFUN is only needed in case of L=1.
MAXIT :	Maximum number of outer iterations, where one iteration corresponds to one formulation and solution of the quadratic programming subproblem, or, alternatively, one evaluation of gradients (e.g. 100).

IPRINT : Specification of the desired output level.

- 0 - No output of the program.
- 1 - Only a final convergence analysis is given.
- 2 - One line of intermediate results is printed in each iteration.
- 3 - More detailed information is printed in each iteration step, e.g. variable, constraint and multiplier values.
- 4 - In addition to 'IPRINT=3', merit function and steplength values are displayed during the line search.

MODE : The parameter specifies the desired version of NLPQLP.

- 0 - Normal execution (reverse communication!).
- 1 - The user wants to provide an initial guess for the multipliers in U and for the Hessian of the Lagrangian function in C.

IOUT : Integer indicating the desired output unit number, i.e. all write-statements start with 'WRITE(IOUT,... '.

IFAIL : The parameter shows the reason for terminating a solution process. Initially IFAIL must be set to zero. On return IFAIL could contain the following values:

- -2 - Compute gradient values w.r.t. the variables stored in first column of X, and store them in DF and DG. Only derivatives for active constraints ACTIVE(J)=.TRUE. need to be computed. Then call NLPQLP again, see below.
- -1 - Compute objective function and all constraint values w.r.t. the variables found in the first L columns of X, and store them in F and G. Then call NLPQLP again, see below.
- 0 - The optimality conditions are satisfied.
- 1 - The algorithm has been stopped after MAXIT iterations.
- 2 - The algorithm computed an uphill search direction.
- 3 - Underflow occurred when determining a new approximation matrix for the Hessian of the Lagrangian.
- 4 - More than MAXFUN function evaluations are required during the line search.
- 5 - Length of a working array is too short. More detailed error information is obtained with 'IPRINT>0'.
- 6 - There are false dimensions, for example M>MMAX, N*geq*NMAX, or MNN2≠M+N+N+2.
- 7 - The search direction is close to zero, but the current iterate is still infeasible.
- 8 - The starting point violates a lower or upper bound.
- >10 - The solution of the quadratic programming subproblem has been terminated with an error message IFQL>0 and IFAIL is set to IFQL+10.

WA(LWA) :	WA is a real working array of length LWA.
LWA :	Length of the real working array WA. LWA must be at least 3/2*NMAX*NMAX+6*MMAX+28*NMAX+100.
KWA(LKWA) :	KWA is an integer working array of length LKWA.
LKWA :	Length of the integer working array KWA. LKWA should be at least MMAX+2*NMAX+20.
ACTIVE(LACTIV) :	The logical array indicates constraints, which NLPQLP considers to be active at the last computed iterate, i.e. G(J,X) is active, if and only if ACTIVE(J)=.TRUE., J=1,...,M.
LACTIV :	Length of the logical array ACTIVE. The length LACTIV of the logical array should be at least 2*MMAX+15.
QP :	External subroutine to solve the quadratic programming subproblem.

The user has to provide functions and gradients in the same program, which executes also NLPQLP, according to the following rules:

1. Choose starting values for the variables to be optimized, and store them in the first column of X.

2. Compute objective and all constraint function values values, store them in F(1) and the first column of G, respectively.

3. Compute gradients of objective function and all constraints, and store them in DF and DG, respectively. The J-th row of DG contains the gradient of the J-th constraint, J=1,...,M.

4. Set IFAIL=0 and execute NLPQLP.

5. If NLPQLP returns with IFAIL=-1, compute objective function values and constraint values for all variables found in the first L columns of X, store them in F (first L positions) and G (first L columns), and call NLPQLP again. If NLPQLP terminates with IFAIL=0, the internal stopping criteria are satisfied. In case of IFAIL>0, an error occurred.

6. If NLPQLP terminates with IFAIL=-2, compute gradient values w.r.t. the variables stored in first column of X, and store them in DF and DG. Only derivatives for active constraints ACTIVE(J)=.TRUE. need to be computed. Then call NLPQLP again.

If analytical derivatives are not available, simultaneous function calls can be used for gradient approximations, for example by forward differences ($2N > L$), two-sided differences ($4N > L \geq 2N$), or even higher order formulae ($L \geq 4N$).

Example:
To give an example how to organize the code, we consider Rosenbrock's post office problem, i.e., test problem TP37 of Hock and Schittkowski [13].

$$
\begin{array}{rl}
 & \min -x_1 x_2 x_3 \\
 & x_1 + 2x_2 + 2x_3 \geq 0 \\
x_1, x_2 \in I\!R: & 72 - x_1 - 2x_2 - 2x_3 \geq 0 \\
 & 0 \leq x_1 \leq 100 \\
 & 0 \leq x_2 \leq 100
\end{array} \tag{19}
$$

The Fortran source code for executing NLPQLP is listed below. Gradients are approximated by forward differences. The function block inserted in the main program, can be replaced by a subroutine call. Also the gradient evaluation is easily exchanged by an analytical one or higher order derivatives.

```
      IMPLICIT NONE
      INTEGER   NMAX,MMAX,LMAX,MNN2X,LWA,LKWA,LACTIV
      PARAMETER (NMAX=4,MMAX=2,LMAX=10)
      PARAMETER (MNN2X = MMAX+NMAX+NMAX+2,
     /          LWA=3*NMAX*NMAX/2+6*MMAX+28*NMAX+100,
     /          LKWA=MMAX+2*NMAX+20,LACTIV=2*MMAX+15)
      INTEGER   KWA(LKWA),KL,N,ME,M,L,MNN2,MAXIT,MAXFUN,IPRINT,
     /          IOUT,MODE,IFAIL,I,J,K,NFUNC
      DOUBLE PRECISION X(NMAX,LMAX),F(LMAX),G(MMAX,LMAX),DF(NMAX),
     /          DG(MMAX,NMAX),U(MNN2X),XL(NMAX),XU(NMAX),C(NMAX,NMAX),
     /          D(NMAX),WA(LWA),ACC,STPMIN,EPS,EPSREL,FBCK,GBCK(MMAX),
     /          XBCK
      LOGICAL   ACTIVE(LACTIV)
      EXTERNAL QL0001
C
      IOUT=6
      ACC=1.0D-9
      STPMIN=1.0E-10
      EPS=1.0D-7
      MAXIT=100
      MAXFUN=10
      IPRINT=2
      N=3
      M=2
      ME=0
      MNN2=M+N+N+2
      DO I=1,N
         X(I,1)=1.0D+1
         XL(I)=0.0
         XU(I)=1.0D+2
      ENDDO
      MODE=0
      IFAIL=0
      NFUNC=0
      L=N
    1 CONTINUE
C=============================================================
C   This is the main block to compute all function values
C   simultaneously, assuming that there are L nodes.
C   The block is executed either for computing a steplength
C   or for approximating gradients by forward differences.
      DO K=1,L
         F(K)=-X(1,K)*X(2,K)*X(3,K)
         G(1,K)=X(1,K) + 2.0*X(2,K) + 2.0*X(3,K)
         G(2,K)=72.0 - X(1,K) - 2.0*X(2,K) - 2.0*X(3,K)
      ENDDO
C=============================================================
      NFUNC=NFUNC+1
      IF (IFAIL.EQ.-1) GOTO 4
```

```
      IF (NFUNC.GT.1) GOTO 3
    2 CONTINUE
      FBCK=F(1)
      DO J=1,M
         GBCK(J)=G(J,1)
      ENDDO
      XBCK=X(1,1)
      DO I=1,N
         EPSREL=EPS*DMAX1(1.0D0,DABS(X(I,1)))
         DO K=2,L
            X(I,K)=X(I,1)
         ENDDO
         X(I,I)=X(I,1)+EPSREL
      ENDDO
      GOTO 1
    3 CONTINUE
      X(1,1)=XBCK
      DO I=1,N
         EPSREL=EPS*DMAX1(1.0D0,DABS(X(I,1)))
         DF(I)=(F(I)-FBCK)/EPSREL
         DO J=1,M
            DG(J,I)=(G(J,I)-GBCK(J))/EPSREL
         ENDDO
      ENDDO
      F=FBCK
      DO J=1,M
         G(J,1)=GBCK(J)
      ENDDO
C
    4 CALL NLPQLP(L,M,ME,MMAX,N,NMAX,MNN2,X,F,G,DF,DG,U,XL,XU,
     /     C,D,ACC,STPMIN,MAXFUN,MAXIT,IPRINT,MODE,IOUT,IFAIL,
     /     WA,LWA,KWA,LKWA,ACTIVE,LACTIV,QL0001)
      IF (IFAIL.EQ.-1) GOTO 1
      IF (IFAIL.EQ.-2) GOTO 2
C
      WRITE(IOUT,1000) NFUNC
 1000 FORMAT('   *** Number of function calls: ',I3)
C
      STOP
      END
```

When applying simultaneous function evaluations with $L = N$, only 20 function calls and 10 iterations are required to get a solution within termination accuracy 10^{-10}. A corresponding call with $L = 1$ would stop after 9 iterations. The following output should appear on screen:

```
   ------------------------------------------------------------------
    START OF THE SEQUENTIAL QUADRATIC PROGRAMMING ALGORITHM
   ------------------------------------------------------------------

    Parameters:
       MODE =  0
       ACC =   0.1000D-08
       MAXFUN =  3
       MAXIT =  100
       IPRINT =   2

    Output in the following order:
       IT    - iteration number
       F     - objective function value
       SCV   - sum of constraint violations
       NA    - number of active constraints
```

```
      I     - number of line search iterations
      ALPHA - steplength parameter
      DELTA - additional variable to prevent inconsistency
      KKT   - Karush-Kuhn-Tucker optimality criterion

    IT         F          SCV     NA  I    ALPHA     DELTA     KKT
   ------------------------------------------------------------------------
     1 -0.10000000D+04  0.00D+00   2  0  0.00D+00  0.00D+00  0.46D+04
     2 -0.10003444D+04  0.00D+00   1  2  0.10D-03  0.00D+00  0.38D+04
     3 -0.33594686D+04  0.00D+00   1  1  0.10D+01  0.00D+00  0.24D+02
     4 -0.33818566D+04  0.16D-09   1  1  0.10D+01  0.00D+00  0.93D+02
     5 -0.34442871D+04  0.51D-08   1  1  0.10D+01  0.00D+00  0.26D+03
     6 -0.34443130D+04  0.51D-08   1  2  0.10D-03  0.00D+00  0.25D+02
     7 -0.34558588D+04  0.19D-08   1  1  0.10D+01  0.00D+00  0.30D+00
     8 -0.34559997D+04  0.00D+00   1  1  0.10D+01  0.00D+00  0.61D-03
     9 -0.34560000D+04  0.00D+00   1  1  0.10D+01  0.00D+00  0.12D-07
    10 -0.34560000D+04  0.00D+00   1  1  0.10D+01  0.00D+00  0.13D-10

    --- Final Convergence Analysis ---

      Objective function value:  F(X) = -0.34560000D+04
      Approximation of solution:  X =
         0.24000000D+02  0.12000000D+02  0.12000000D+02
      Approximation of multipliers:  U =
         0.00000000D+00  0.14400000D+03  0.00000000D+00  0.00000000D+00
         0.00000000D+00  0.00000000D+00  0.00000000D+00  0.00000000D+00
      Constraint values:  G(X) =
         0.72000000D+02  0.35527137D-13
      Distance from lower bound:  XL-X =
        -0.24000000D+02 -0.12000000D+02 -0.12000000D+02
      Distance from upper bound:  XU-X =
         0.76000000D+02  0.88000000D+02  0.88000000D+02
      Number of function calls:     NFUNC =  10
      Number of gradient calls:     NGRAD =  10
      Number of calls of QP solver: NQL   =  10

   *** Number of function calls:  20
```

In case of $L = 1$, NLPQLP is identical to NLPQL and stops after 9 iterations. The corresponding sequential implementation of the main program is as follows:

```
      IMPLICIT NONE
      INTEGER   NMAX,MMAX,LMAX,MNN2X,LWA,LKWA,LACTIV
      PARAMETER (NMAX=4,MMAX=2)
      PARAMETER (MNN2X = MMAX+NMAX+NMAX+2,
     /           LWA=3*NMAX*NMAX/2+6*MMAX+28*NMAX+100,
     /           LKWA=MMAX+2*NMAX+20,LACTIV=2*MMAX+15)
      INTEGER   KWA(LKWA),KL,N,ME,M,L,MNN2,MAXIT,MAXFUN,IPRINT,
     /          IOUT,MODE,IFAIL,I,J,K
      DOUBLE PRECISION X(NMAX),F,G(MMAX),DF(NMAX),
     /          DG(MMAX,NMAX),U(MNN2X),XL(NMAX),XU(NMAX),C(NMAX,NMAX),
     /          D(NMAX),WA(LWA),ACC,STPMIN,EPS,EPSREL,FBCK,GBCK(MMAX)
      LOGICAL   ACTIVE(LACTIV)
      EXTERNAL QL0001
C
      IOUT=6
      ACC=1.0D-9
      STPMIN=0.0
      EPS=1.0D-7
      MAXIT=100
      MAXFUN=10
      IPRINT=2
      N=3
      M=2
```

```
      ME=0
      MNN2=M+N+N+2
      DO I=1,N
         X(I)=1.0D+1
         XL(I)=0.0
         XU(I)=1.0D+2
      ENDDO
      MODE=0
      IFAIL=0
      L=1
      I=0
    1 CONTINUE
C============================================================
C   This is the main block to compute all function values.
C   The block is executed either for computing a steplength
C   or for approximating gradients by forward differences.
      F=-X(1)*X(2)*X(3)
      G(1)=X(1) + 2.0*X(2) + 2.0*X(3)
      G(2)=72.0 - X(1) - 2.0*X(2) - 2.0*X(3)
C============================================================
      IF (IFAIL.EQ.-1) GOTO 4
      IF (I.GT.0) GOTO 3
    2 CONTINUE
      FBCK=F
      DO J=1,M
         GBCK(J)=G(J)
      ENDDO
      I=0
    5 I=I+1
      EPSREL=EPS*DMAX1(1.0D0,DABS(X(I)))
      X(I)=X(I)+EPSREL
      GOTO 1
    3 CONTINUE
      DF(I)=(F-FBCK)/EPSREL
      DO J=1,M
         DG(J,I)=(G(J)-GBCK(J))/EPSREL
      ENDDO
      X(I)=X(I)-EPSREL
      IF (I.LT.N) GOTO 5
      F=FBCK
      DO J=1,M
         G(J)=GBCK(J)
      ENDDO
C
    4 CALL NLPQLP(L,M,ME,MMAX,N,NMAX,MNN2,X,F,G,DF,DG,U,XL,XU,
     /     C,D,ACC,STPMIN,MAXFUN,MAXIT,IPRINT,MODE,IOUT,IFAIL,
     /     WA,LWA,KWA,LKWA,ACTIVE,LACTIV,QL0001)
      IF (IFAIL.EQ.-1) GOTO 1
      IF (IFAIL.EQ.-2) GOTO 2
C
      STOP
      END
```

7 Summary

We present a modification of an SQP algorithm designed for execution under a parallel computing environment (SPMD). Under the assumption that objective functions and constraints are executed on different machines, a parallel line search procedure is proposed. Thus, the SQP algorithm is executable under a distributed system, where parallel function calls are exploited for line search and gradient approximations.

The approach is outlined, the usage of the program is documented, and some numerical tests are performed. It is shown that there are no significant performance differences between sequential and parallel line searches, if the number of parallel processors is sufficiently large. In both cases, about the same number of iterations is performed, and the number of successfully solved problems is also comparable. The test results are obtained by a collection of 306 academic and real-life examples.

By a series of further tests, it is shown how the code behaves for 6 different gradient approximations under additional random noise added to the model functions, to simulate realistic situations arising in practical applications. If a sufficiently large number of parallel processors is available, it is recommended to apply higher order approximation formulae instead of forward differences. Linear and quadratic approximations perform well in case of large round-off errors.

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